(FILE 'HOME' ENTERED AT 13:03:30 ON 21 MAY 1998)

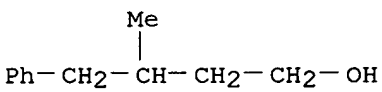
FILE 'REGISTRY' ENTERED AT 13:03:36 ON 21 MAY 1998

L1 SCREEN 1992
L2 SCREEN 2016
L3 SCREEN 2021
L4 SCREEN 1929
L5 SCREEN 1839
L6 SCREEN 963 AND 1006 AND 1051
L7 STRUCTURE UPLOADED
L8 QUE L7 AND L6 NOT L1 NOT L2 NOT L3 NOT L4 NOT L5
L9 0 S L8
L10 1 S L8 FULL

FILE 'CAPLUS' ENTERED AT 13:04:30 ON 21 MAY 1998
L11 3 S L10

=> d bib ab hitstr 1-3

L11 ANSWER 1 OF 3 CAPLUS COPYRIGHT 1998 ACS
AN 1997:706261 CAPLUS
DN 128:3495
TI Enantioselective carbolithiation of .beta.-alkylated styrene
AU Norsikian, Stephanie; Marek, Ilane; Normant, Jean-F.
CS Laboratoire de Chimie des Organoelements, associe au C.N.R.S., Universite P. et M. Curie, Paris, 75252, Fr.
SO Tetrahedron Lett. (1997), 38(43), 7523-7526
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
OS CASREACT 128:3495
AB Stoichiometric or catalytic amts. of (-)-sparteine serve as promoter for enantioselective carbolithiation of .beta.-alkylated, non-functionalized styrene. For example, the carbolithiation of (E)-(1-butenyl)benzene in the presence of (-)-sparteine gave (S)-(2-ethylhexyl)benzene which was converted to the known (S)-3-ethyl-1-heptanol.
IT **34126-21-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective carbolithiation of .beta.-alkylated styrene)
RN 34126-21-1 CAPLUS
CN Benzenebutanol, .gamma.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 2 OF 3 CAPLUS COPYRIGHT 1998 ACS
AN 1972:564829 CAPLUS
DN 77:164829
TI Stereoselectivity in the carbonyl insertion reaction between tetracarbonyldichlorodirhodium and substituted cyclopropanes

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Trying 9351006...Open

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


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                  Available
 NEWS  3  May 18  Variable SDI Frequencies Now Available in EMBAL

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FILE 'HOME' ENTERED AT 12:15:06 ON 04 JUN 1998

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DICTIONARY FILE UPDATES:  3 JUN  98  HIGHEST RN 206111-35-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 14, 1998

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 963 AND 1006 AND 1051

L1    SCREEN CREATED
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L2      STRUCTURE UPLOADED

=> que L2 AND L1

L3   QUE L2 AND L1

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=> screen 964 AND 1006 AND 1051

L4    SCREEN CREATED

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L5      STRUCTURE UPLOADED

=> que L5 AND L4

L6   QUE L5 AND L4

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=> screen 963 AND 1006 AND 1051

L7    SCREEN CREATED

=>
Uploading c:\stnexp4\queries\860007.str

L8      STRUCTURE UPLOADED

=> que L8 AND L7

L9   QUE L8 AND L7

=> query

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L10  QUE L2 OR L5 OR L8

=> d l10

L10 HAS NO ANSWERS
L2                STR
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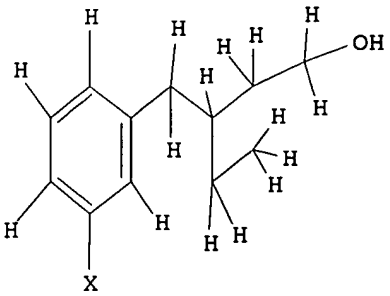

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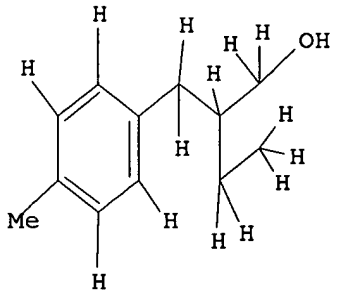
L5 STR



Structure attributes must be viewed using STN Express query preparation.
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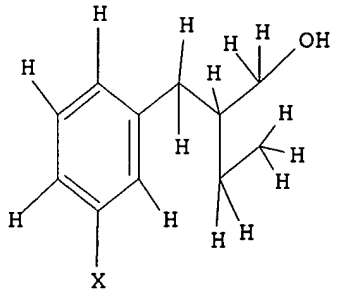

Structure attributes must be viewed using STN Express query preparation.
L10 QUE L2 OR L5 OR L8

=> s l10

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100.0% PROCESSED 813 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 14550 TO 17970
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L2 OR L5 OR L8

=> s l10 sss full

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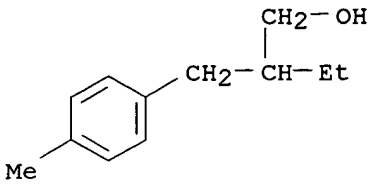
100.0% PROCESSED 16383 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.09

L12 1 SEA SSS FUL L2 OR L5 OR L8

=> d 1 sub bib

L12 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1998 ACS
RN 156054-37-4 REGISTRY
CN Benzenepropanol, .beta.-ethyl-4-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 O
SR CA
LC STN Files: CA, CAPLUS



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

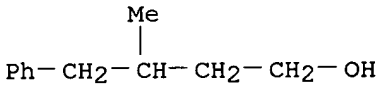
REFERENCE 1

AN 121:82711 CA
TI 3-(4-methylphenyl)-2-(ar)alkylpropanals, their preparation and fragrance application
IN Kleemiss, Wolfgang; Kalz, Thomas
PA Huels AG, Germany
SO Ger. Offen., 6 pp.
CODEN: GWXXBX
PI DE 4236887 A1 940505
AI DE 92-4236887 921031
DT Patent
LA German

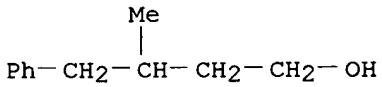
REFERENCE 2

AN 121:82702 CA
TI 3-(4-methylphenyl)-2-(ar)alkylpropan-1-ols, process for their preparation and use in fragrance applications
IN Kleemiss, Wolfgang; Kaufhold, Manfred
PA Huels AG, Germany
SO Ger. Offen., 6 pp.
CODEN: GWXXBX
PI DE 4236889 A1 940505
AI DE 92-4236889 921031
DT Patent
LA German

AU McQuillin, F. J.; Powell, K. G.
CS Dep. Org. Chem., Univ. Newcastle upon Tyne, Newcastle-upon-Tyne, Engl.
SO J. Chem. Soc., Dalton Trans. (1972), (19), 2129-33
CODEN: JCDTBI
DT Journal
LA English
AB The in-sertion reaction between [Rh(CO)2Cl]2 and phenyl- or benzyl-cyclopropane, or bicyclo [4.1.0]heptane was examd. and the struc-tures of the products deduced by NaBH4 redn.; e.g., [Rh(CO)2Cl]2 with phenylcyclopropane at 60.degree. gave the 1-chloro-1-carbonyl-5-phenylrhodacyclopentan-2-one (I) which gave Ph(CH2)4OH on redn. Prolonged heating with [Rh(CO)2Cl]2 caused isomeriza-tion of the cyclopropane to olefin.
IT **34126-21-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 34126-21-1 CAPLUS
CN Benzenebutanol, .gamma.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 3 OF 3 CAPLUS COPYRIGHT 1998 ACS
AN 1971:529929 CAPLUS
DN 75:129929
TI Reactions of cyclopropanes with dicarbonylchlororhodium. Carbonyl insertion and isomerization
AU McQuillin, F. J.; Powell, K. G.
CS Dep. Org. Chem., Univ. Newcastle-upon-Tyne, Newcastle-upon-Tyne, Engl.
SO J. Chem. Soc. D. (1971), (16), 931-2
CODEN: CCJDAO
DT Journal
LA English
AB With [Rh(CO)2Cl]2, phenylcyclopropane underwent stereoselective ring fission to give the carbonyl inserted product (I) and PhCH:CHMe; benzylcyclopropane and bicyclo[4.1.0]heptane reacted similarly.
IT **34126-21-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 34126-21-1 CAPLUS
CN Benzenebutanol, .gamma.-methyl- (9CI) (CA INDEX NAME)



CN **Formaldehyde, compd. with [S-(R*,R*)]-.beta.-amino-.alpha.-(chloromethyl)benzenepropanol (1:1) (9CI)** (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanol, .beta.-amino-.alpha.-(chloromethyl)-, [S-(R*,R*)]-, compd. with formaldehyde (1:1) (9CI)

FS STEREOSEARCH

MF C10 H14 Cl N O . C H2 O

SR CA

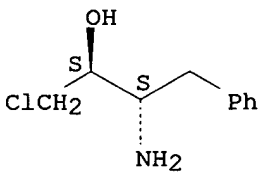
LC STN Files: CA, CAPLUS

CM 1

CRN 160232-67-7

CMF C10 H14 Cl N O

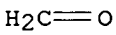
Absolute stereochemistry.



CM 2

CRN 50-00-0

CMF C H2 O



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 126:31265 CA

TI Preparation of tetrahydrofuran-containing sulfonamide inhibitors of aspartyl protease for treatment of HIV infection.

IN Tung, Roger D.

PA Vertex Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 105 pp
CODEN: PIXXD2

PI WO 9633184 A1 961024

DS W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, NL, PT, SE

AI WO 96-US5475 960418

PRAI US 95-424819 950419

DT Patent

LA English

=> d 2 sub bib

L13 ANSWER 2 OF 6 REGISTRY COPYRIGHT 1998 ACS

RN 186497-72-3 REGISTRY

CN Benzenepropanol, 4-bromo-.beta.-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

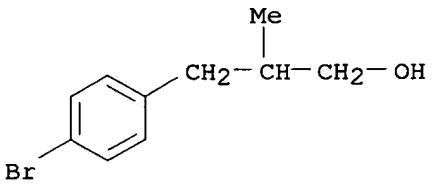
CN 2-Methyl-3-(4-bromophenyl)-1-propanol

CN **4-Bromo-.beta.-methylbenzenepropanol**

FS 3D CONCORD

MF C10 H13 Br O

SR CA
LC STN Files: CA, CAPLUS



3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 127:50629 CA
TI Preparation of substituted biphenylsulfonamide derivatives as endothelin antagonists
IN Marugesan, Natesan; Barrish, Joel C.; Lloyd, John
PA Bristol-Myers Squibb Company, Japan
SO Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
PI JP 09124620 A2 970513 Heisei
AI JP 96-262859 961003
PRAI US 95-60007032 951011
DT Patent
LA Japanese

REFERENCE 2

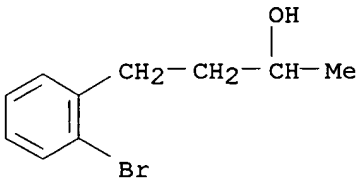
AN 126:343561 CA
TI Preparation of N-isoxazolyl-biphenylsulfonamides as endothelin antagonists
IN Murugesan, Natesan; Barrish, Joel C.; Lloyd, John
PA Bristol-Myers Squibb Company, USA
SO Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
PI EP 768305 A1 970416
DS R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
AI EP 96-116095 961008
PRAI US 95-7032 951011
DT Patent
LA English

REFERENCE 3

AN 126:144291 CA
TI N-pyrazinyl-2-phenyl-3-pyridinesulfonamides and analogs endothelin receptor antagonists
IN Bradbury, Robert Hugh; Butlin, Roger John; James, Roger
PA Zeneca Limited, UK
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
PI WO 9640681 A1 961219
DS W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 96-GB1295 960603
PRAI GB 95-11507 950607
GB 95-19666 950927
DT Patent
LA English

=> d 5-6 sub bib

L13 ANSWER 5 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 67130-96-5 REGISTRY
CN Benzenepropanol, 2-bromo-.alpha.-methyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **2-Bromo-.alpha.-methylbenzenepropanol**
FS 3D CONCORD
MF C10 H13 Br O
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CJACS
(*File contains numerically searchable property data)



5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 128:282703 CA
TI Preparation of aryl ethers
IN Buchwald, Stephen L.; Wolfe, John P.; Palucki, Michael
PA Massachusetts Institute of Technology, USA; Buchwald, Stephen L.; Wolfe, John P.; Palucki, Michael
SO PCT Int. Appl., 72 pp.
CODEN: PIXXD2
PI WO 9815515 A1 980416
DS W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 97-US18719 971010
PRAI US 96-728449 961010
DT Patent
LA English

REFERENCE 2

AN 126:7946 CA
TI Synthesis of Oxygen Heterocycles via a Palladium-Catalyzed C-O Bond-Forming Reaction
AU Palucki, Michael; Wolfe, John P.; Buchwald, Stephen L.
CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SO J. Am. Chem. Soc. (1996), 118(42), 10333-10334
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English

REFERENCE 3

AN 106:195544 CA
TI Lithium-halogen exchange-initiated cyclization reactions. 3. Intramolecular conjugate addition reactions of unsaturated acylphosphoranes
AU Cooke, Manning P., Jr.; Widener, Rexford K.
CS Dep. Chem., Washington State Univ., Pullman, WA, 99164, USA

SO J. Org. Chem. (1987), 52(8), 1381-96
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English

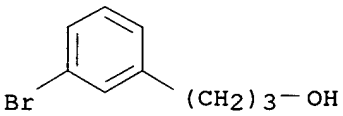
REFERENCE 4

AN 96:6277 CA
TI Selective halogen-lithium exchange in some secondary and tertiary (bromophenyl)alkyl halides
AU Parham, William E.; Bradsher, Charles K.; Reames, David C.
CS Paul M. Gross Chem. Lab., Duke Univ., Durham, NC, 27706, USA
SO J. Org. Chem. (1981), 46(23), 4804-6
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English

REFERENCE 5

AN 89:107234 CA
TI Nucleophilic aromatic substitution by organostannylsodiums. A second-order reaction displaying a solvent cage effect
AU Wursthorn, Karl R.; Kuivila, Henry G.; Smith, Gary F.
CS Dep. Chem., State Univ. New York, Albany, N. Y., USA
SO J. Am. Chem. Soc. (1978), 100(9), 2779-89
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English

L13 ANSWER 6 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 65537-54-4 REGISTRY
CN Benzenepropanol, 3-bromo- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-(3-Bromophenyl)-1-propanol
CN **3-Bromobenzenepropanol**
FS 3D CONCORD
MF C9 H11 Br O
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CJACS, IFICDB, IFIPAT, IFIUDB, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



10 REFERENCES IN FILE CA (1967 TO DATE)
10 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 128:114790 CA
TI Preparation of biphenylamidines as anticoagulants for inhibition and treatment of thrombus and embolus
IN Nomoto, Takashi; Kawamoto, Hiroshi; Sato, Sadashi; Honma, Mitsuki; Miyaji, Mitsuru; Takaenoki, Yoko
PA Banyu Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 26 pp.
CODEN: JKXXAF
PI JP 10001467 A2 980106 Heisei
AI JP 96-174219 960613
DT Patent
LA Japanese

REFERENCE 2

AN 127:358794 CA
TI Aminoisoquinolines and aminothienopyridine derivatives and their use

as anti-inflammatory agents
IN Hamley, Peter; Macdonald, James; Matz, James; Tinker, Alan
PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag; Hamley, Peter; Macdonald, James; Matz, James; Tinker, Alan
SO PCT Int. Appl., 92 pp.
CODEN: PIXXD2
PI WO 9738977 A1 971023
DS W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 97-SE589 970409
PRAI GB 96-7717 960413
GB 96-8678 960426
GB 96-10892 960524
DT Patent
LA English

REFERENCE 3

AN 127:26625 CA
TI Preparation of liquid crystal cyclohexylbenzene compounds containing halogen and alkenyl groups and liquid crystal composition
IN Haseba, Yasuhiro; Koga, Koji; Matsui, Shuichi; Miyazawa, Kazutoshi; Sekiguchi, Yasuko; Nakagawa, Etsuo
PA Chisso Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 97 pp.
CODEN: JKXXAF
PI JP 09077703 A2 970325 Heisei
AI JP 95-258186 950911
DT Patent
LA Japanese

REFERENCE 4

AN 120:54536 CA
TI Oxazole and imidazole derivatives as prostaglandin analogs and thromboxane receptor antagonists
IN Misra, Raj N.; Das, Jagabandhu; Hall, Steven E.; Han, Wen Ching; Sher, Philip M.; Stein, Philip D.
PA Squibb, E. R., and Sons, Inc., USA
SO Eur. Pat. Appl., 92 pp.
CODEN: EPXXDW
PI EP 536713 A1 930414
DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
AI EP 92-117099 921007
PRAI US 91-772830 911007
DT Patent
LA English

REFERENCE 5

AN 111:214378 CA
TI Displacements at the nitrogen of lithioalkoxylamides by organometallic reagents
AU Beak, Peter; Selling, Gordon W.
CS Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
SO J. Org. Chem. (1989), 54(23), 5574-80
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English

REFERENCE 6

AN 96:98909 CA
TI Isolation and identification of mercapturic acids of cinnamic

aldehyde and cinnamyl alcohol from urine of female rats
AU Delbressine, L. P. C.; Klippert, P. J. M.; Reuvers, J. T. A.; Seutter-Berlage, F.
CS Dep. Pharmacol., Univ. Nijmegen, Nijmegen, NL-6500 HB, Neth.
SO Arch. Toxicol. (1981), 49(1), 57-64
CODEN: ARTODN; ISSN: 0340-5761
DT Journal
LA English

REFERENCE 7

AN 93:132142 CA
TI Methylenecyclopentane derivatives
IN Morton, Douglas R., Jr.
PA Upjohn Co., USA
SO U.S., 21 pp. Division of U.S. Ser. No. 764,332 abandoned.
CODEN: USXXAM
PI US 4195178 800325
AI US 76-691792 760601
DT Patent
LA English

REFERENCE 8

AN 92:146342 CA
TI Methylenecyclopentane derivatives
IN Morton, Douglas R., Jr.
PA Upjohn Co., USA
SO U.S., 22 pp.
CODEN: USXXAM
PI US 4181798 800101
AI US 76-691792 760601
DT Patent
LA English

REFERENCE 9

AN 89:108349 CA
TI 4,5,6-Trinor-3,7-inter-m-phenylene prostaglandin F1.alpha. analogs
IN Nelson, Norman A.
PA Upjohn Co., USA
SO U.S., 36 pp.
CODEN: USXXAM
PI US 4084058 780411
AI US 75-604158 750813
DT Patent
LA English

REFERENCE 10

AN 88:104766 CA
TI Optically active phenyl derivatives of prostaglandins
PA Upjohn Co., USA
SO Neth. Appl., 88 pp.
CODEN: NAXXAN
PI NL 7608823 770215
PRAI US 75-604158 750813
DT Patent
LA Dutch

=> file uspat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	29.72	29.87

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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 2 Jun 1998 (19980602/PD)

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FILE LAST UPDATED: 3 Jun 1998 (19980603/ED)
HIGHEST PATENT NUMBER: US5761741
CA INDEXING IS CURRENT THROUGH 3 Jun 1998 (19980603/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 2 Jun 1998 (19980602/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Mar 1998
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 1998

>>> Page images are available for patents from 1/1/95.  Current     <<<
>>> week patent text is typically loaded by Thursday morning and    <<<
>>> page images are available for display by the end of the day.    <<<
>>> Image data for the /FA field are available the following week.  <<<

>>> Complete CA file indexing for chemical patents (or equivalents) <<<
>>> is included in file records.  A thesaurus is available for the  <<<
>>> USPTO Manual of Classifications in the /NCL, /INCL, and /RPCL   <<<
>>> fields.  This thesaurus includes catchword terms from the       <<<
>>> USPTO/MOC subject headings and subheadings.  Thesauri are also  <<<
>>> available for the WIPO International Patent Classification      <<<
>>> (IPC) Manuals, editions 1-6, in the /IC1, /IC2, /IC3, /IC4,     <<<
>>> /IC5, and /IC (/IC6) fields, respectively.  The thesauri in     <<<
>>> the /IC5 and /IC fields include the corresponding catchword     <<<
>>> terms from the IPC subject headings and subheadings.            <<<

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d his


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L3               QUE L2 AND L1
L4               SCREEN 963 AND 1006 AND 1051
L5               STRUCTURE UPLOADED
L6               QUE L5 AND L4
L7               STRUCTURE UPLOADED
L8               QUE L7
L9               QUERY L2 OR L5 NOT L7
L10            0 SEARCH L9
L11         6599 S BENZENEPROPANOL
L12      2590878 S CHLORO OR BROMO
L13            6 S L12(2W)L11

     FILE 'USPATFULL' ENTERED AT 14:14:35 ON 05 JUN 1998

=> s l13

L14            5 L13

=> d 1


L14  ANSWER 1 OF 5  USPATFULL
AN     1998:22250  USPATFULL
TI     THF-containing sulfonamide inhibitors of aspartyl protease
IN     Tung, Roger D., Arlington, MA, United States
PA     Vertex Pharmaceuticals Incorporated, Cambridge, MA, United States
       (U.S. corporation)
PI     US 5723490  980303
AI     US 95-424819  950419 (8)
RLI    Continuation-in-part of Ser. No. US 95-393460, filed on 23 Feb
       1995, now abandoned which is a continuation-in-part of Ser. No. US
       93-142327, filed on 24 Nov 1993, now patented, Pat. No. US 5585397
       which is a continuation-in-part of Ser. No. US 92-941982, filed on
       8 Sep 1992, now abandoned
DT     Utility
LN.CNT 2481
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INCL INCLM: 514/478.000
INCLS: 514/477.000; 514/588.000; 514/050.000
NCL NCLM: 514/478.000
NCLS: 514/050.000; 514/477.000; 514/588.000
IC [6]
ICM: A61K031-27
ICS: A61K031-17; A61K031-70
EXF 514/50; 514/478; 514/497; 514/588
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d 1 hit

L14 ANSWER 1 OF 5 USPATFULL
IT 3217-94-5P, Cyclopentanecarboxamide 24924-72-9P 62992-68-1P
88915-26-8P 95798-23-5P 120278-07-1P 159141-66-9P
160230-41-1P 160231-30-1P 160231-33-4P 160232-08-6P
160232-45-1P 160232-54-2P 160232-56-4P 160232-62-2P
160232-63-3P **160232-68-8P** 160232-69-9P 160232-70-2P
160232-71-3P 160232-72-4P 160232-91-7P 160232-99-5P
160233-19-2P 160233-23-8P 169814-97-5P 184357-17-3P
184357-20-8P 184357-21-9P 184357-36-6P 184357-37-7P
184357-38-8P 184357-39-9P 184357-40-2P 184357-41-3P
184357-42-4P 186463-17-2P 186463-23-0P 203851-90-5P
203851-91-6P 203851-92-7P 203851-93-8P 203851-95-0P
203851-96-1P 203851-97-2P 203851-98-3P 203851-99-4P
203852-00-0P 203852-01-1P 203852-02-2P 203852-03-3P
203852-04-4P 203852-05-5P 203852-06-6P 203852-07-7P
203852-08-8P 203852-09-9P 203852-10-2P 203852-11-3P
203852-12-4P
(prepn. of THF-contg. sulfonamides as inhibitors of aspartyl protease)

=> d 2-4

L14 ANSWER 2 OF 5 USPATFULL
AN 96:116404 USPATFULL
TI Sulfonamide inhibitors of aspartyl protease
IN Tung, Roger D., Arlington, MA, United States
Murcko, Mark A., Holliston, MA, United States
Bhisetti, Govinda R., Lexington, MA, United States
PA Vertex Pharmaceuticals, Incorporated, Cambridge, MA, United States (U.S. corporation)
PI US 5585397 961217
WO 9405639 940317
AI US 93-142327 931124 (8)
WO 93-US8458 930907
930907 PCT 371 date
930907 PCT 102(e) date
RLI Continuation-in-part of Ser. No. US 92-941982, filed on 8 Sep 1992, now abandoned
DT Utility
LN.CNT 7153
INCL INCLM: 514/473.000
INCLS: 514/464.000; 549/475.000; 549/448.000; 546/169.000
NCL NCLM: 514/473.000
NCLS: 514/464.000; 546/169.000; 549/448.000; 549/475.000
IC [6]
ICM: C07D407-12
ICS: C07D307-20; A61K031-34
EXF 546/169; 549/475; 549/448; 514/473; 514/464
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L14 ANSWER 3 OF 5 USPATFULL
AN 80:15170 USPATFULL
TI Methylenecyclopentane derivatives
IN Morton, Jr., Douglas R., Portage, MI, United States
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)

PI US 4195178 800325
AI US 78-947689 781002 (5)
RLI Division of Ser. No. US 77-764332, filed on 31 Jan 1977, now abandoned which is a continuation-in-part of Ser. No. US 76-691792, filed on 1 Jun 1976, now abandoned
DT Utility
LN.CNT 1404
INCL INCLM: 542/426.000
INCLS: 542/429.000; 568/838.000; 260/347.800; 260/333.000
NCL NCLM: 549/214.000
NCLS: 549/312.000; 549/346.000; 549/415.000; 549/417.000; 549/421.000; 549/472.000; 549/473.000; 549/475.000; 549/476.000; 568/838.000
IC [2]
ICM: C07D407-08
ICS: C07D407-14
EXF 568/838; 542/426
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L14 ANSWER 4 OF 5 USPATFULL
AN 80:999 USPATFULL
TI Methylenecyclopentane derivatives
IN Morton, Jr., Douglas R., Portage, MI, United States
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 4181798 800101
AI US 78-947688 781002 (5)
RLI Continuation-in-part of Ser. No. US 77-764332, filed on 31 Jan 1977, now abandoned which is a continuation-in-part of Ser. No. US 76-691792, filed on 1 Jun 1976, now abandoned
DT Utility
LN.CNT 1540
INCL INCLM: 542/426.000
INCLS: 568/838.000
NCL NCLM: 549/214.000
NCLS: 549/346.000; 549/415.000; 549/472.000; 549/473.000; 568/838.000
IC [2]
ICM: C07D407-08
EXF 568/838; 542/426
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d 2-4 hit

L14 ANSWER 2 OF 5 USPATFULL
IT 1080-11-1P 1828-66-6P, 4-Morpholinesulfonyl chloride 4295-99-2P 6053-81-2P, Aminomethylcyclopentane 23905-46-6P 25506-37-0P 30293-86-8P 32939-32-5P 35856-62-3P, 1-Piperidinesulfonyl chloride 52206-05-0P 52665-49-3P, 3-Furansulfonyl chloride 54981-39-4P 87001-32-9P, 4-Benzyloxybenzenesulfonyl chloride 102522-17-8P 114322-14-4P, 2,1,3-Benzoxadiazole-4-sulfonyl chloride 115010-10-1P, 1,3-Benzodioxole-5-sulfonyl chloride 115010-11-2P, 2,3-Dihydrobenzofuran-5-sulfonyl chloride 116586-32-4P 130290-79-8P 132682-22-5P 132682-23-6P 134807-06-0P 134807-20-8P 138499-08-8P 143224-83-3P 159006-03-8P 159006-20-9P 159141-66-9P 160231-97-0P 160231-98-1P 160231-99-2P 160232-00-8P 160232-01-9P 160232-02-0P 160232-03-1P 160232-05-3P 160232-06-4P 160232-08-6P 160232-09-7P 160232-10-0P 160232-11-1P 160232-12-2P 160232-13-3P 160232-14-4P 160232-15-5P, 2,1,3-Benzoxadiazole-4-sulfonic acid 160232-17-7P 160232-18-8P 160232-19-9P, 2,1,3-Benzoxadiazole-5-thiol 160232-20-2P, 2,1,3-Benzoxadiazole-5-sulfonyl chloride 160232-22-4P 160232-23-5P 160232-24-6P 160232-25-7P 160232-26-8P 160232-27-9P 160232-28-0P 160232-29-1P 160232-30-4P 160232-31-5P 160232-32-6P 160232-33-7P 160232-34-8P 160232-36-0P 160232-37-1P 160232-38-2P 160232-39-3P 160232-40-6P 160232-41-7P 160232-42-8P 160232-43-9P 160232-44-0P 160232-45-1P 160232-46-2P 160232-47-3P

160232-48-4P 160232-49-5P 160232-50-8P 160232-51-9P
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160232-60-0P 160232-61-1P 160232-62-2P 160232-63-3P
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184357-14-0P 184357-17-3P 186463-21-8P 186463-22-9P
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186463-27-4P 186463-28-5P 186463-29-6P 186463-30-9P
186463-31-0P 186463-32-1P 186463-33-2P 186463-35-4P
186463-37-6P 186463-39-8P
(prepn. of sulfonamide inhibitors of aspartyl protease)

L14 ANSWER 3 OF 5 USPATFULL
IT 591-20-8 **65537-54-4**
(silylation of)

L14 ANSWER 4 OF 5 USPATFULL
IT 591-20-8 **65537-54-4**
(silylation of)

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.79	36.66

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L3   QUE L2 AND L1

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PROJECTED ITERATIONS:         2725 TO     4315
PROJECTED ANSWERS:               9 TO      360

L4            9 SEA SSS SAM L2 AND L1

=> d 1 sub bib


L4   ANSWER 1 OF 9  REGISTRY  COPYRIGHT 1998 ACS
RN   182686-37-9  REGISTRY
CN   Propanedioic acid, ([1,1'-biphenyl]-2-ylmethyl)methyl-, diethyl
     ester (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C21 H24 O4
SR   CA
LC   STN Files:   CA, CAPLUS
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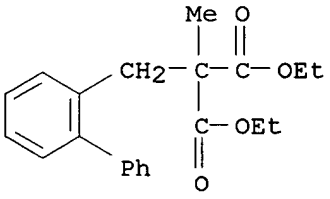


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                1 REFERENCES IN FILE CA (1967 TO DATE)
                1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE  1

AN   125:276900  CA
TI   Manufacture of .alpha.-olefin polymers in the presence of highly
     active catalysts containing transition metal complexes and
     aluminoxanes
IN   Sugano, Toshihiko
PA   Mitsubishi Chem Corp, Japan
SO   Jpn. Kokai Tokkyo Koho, 17 pp.
     CODEN: JKXXAF
PI   JP 08208733 A2  960813  Heisei
AI   JP 95-14440  950131
DT   Patent
LA   Japanese

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L5    SCREEN CREATED
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L3 MAY NOT BE USED HERE
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=> query

ENTER LOGIC EXPRESSION OR (END):l2 not l5

L6 QUE L2 NOT L5

=> s l6

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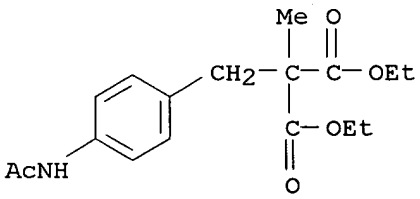
100.0% PROCESSED 65 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 817 TO 1783
PROJECTED ANSWERS: 6 TO 266

L7 6 SEA SSS SAM L2 NOT L5

=> d 1 sub bib

L7 ANSWER 1 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 144872-09-3 REGISTRY
CN Propanedioic acid, [[4-(acetylamino)phenyl]methyl]methyl-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H23 N O5
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



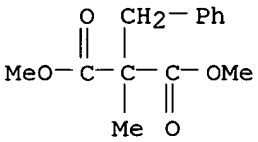
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 118:101720 CA
TI Preparation of 8-substituted purines as selective adenosine receptor agents
IN Peet, Norton P.; Dudley, Mark W.; Lentz, Nelsen L.
PA Merrell Dow Pharmaceuticals, Inc., USA
SO Eur. Pat. Appl., 42 pp.
    CODEN: EPXXDW
PI EP 503563 A2 920916
DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE
AI EP 92-104089 920310
PRAI US 91-667943 910312
DT Patent
LA English

=> d 2 sub bib

L7 ANSWER 2 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 120681-58-5 REGISTRY
CN Propanedioic acid, methyl(phenylmethyl)-, dimethyl ester, (R)- (9CI) (CA INDEX NAME)
MF C13 H16 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



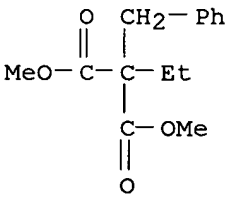
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 110:210971 CA
TI Enzymic manufacture of optically active malonic acid monoesters from the corresponding diesters
IN Hult, Karl; Boutelje, John; Gatenbeck, Sten; Norin, Torbjoern; Bjoerkling, Fredrik
PA Swed.
SO Swed., 11 pp.
CODEN: SSXXAY
PI SE 453599 B 880215
AI SE 85-2051 850426
DT Patent
LA Swedish

=> d 3 sub bib

L7 ANSWER 3 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 113741-14-3 REGISTRY
CN Propanedioic acid, ethyl(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H18 O4
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

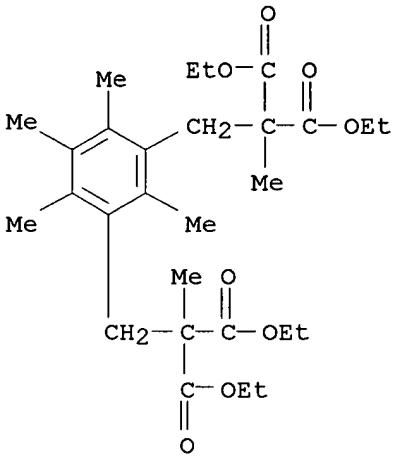
REFERENCE 1

AN 108:146043 CA
TI Computer graphics as a tool for the prediction of the stereoselectivity of enzyme catalyzed reactions. .alpha.-Chymotrypsin catalyzed hydrolysis of substituted propanedioic acid diesters
AU Bjoerkling, Fredrik; Norin, Torbjoern; Szmulik, Peter; Boutelje,

John; Hult, Karl; Kraulis, Per
CS Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.
SO Biocatalysis (1987), 1(1), 87-98, 2 plates
CODEN: BIOCED; ISSN: 0886-4454
DT Journal
LA English

=> d 4 sub bib

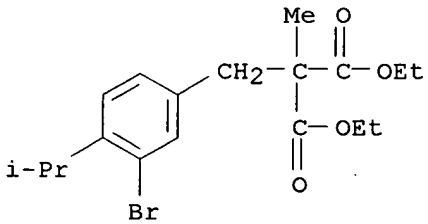
L7 ANSWER 4 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 97355-07-2 REGISTRY
CN Malonic acid, [(tetramethyl-m-phenylene)dimethylene]bis[methyl-, tetraethyl ester (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H42 O8
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d 5 sub bib

L7 ANSWER 5 OF 6 REGISTRY COPYRIGHT 1998 ACS
RN 70146-89-3 REGISTRY
CN Propanedioic acid, [[3-bromo-4-(1-methylethyl)phenyl]methyl]methyl-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H25 Br O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXLIT
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 90:179912 CA

TI Quantitative relationships between structure and fibrinolytic activity in the series of .alpha.-methyl-.beta.-arylpropionic acids
AU Kuchar, Miroslav; Rejholec, Vaclav; Roubal, Zdenek; Nemecek, Oldrich
CS Res. Inst. Pharm. Biochem., Prague, Czech.
SO Collect. Czech. Chem. Commun. (1979), 44(1), 183-93
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English

=> s l6 sss full

FULL SEARCH INITIATED 15:47:16
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SEARCH TIME: 00.00.02

L8 128 SEA SSS FUL L2 NOT L5

=> file ca

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	127.02	127.17

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1967 - 2 Jun 1998 (980602/ED) VOL 128 ISS 23

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8

L9 106 L8

=> s arylpropanol? or benzenepropanol? or phenylpropanol?

42 ARYLPROPANOL?
195 BENZENEPROPANOL?
1488 PHENYLPROPANOL?
L10 1713 ARYLPROPANOL? OR BENZENEPROPANOL? OR PHENYLPROPANOL?

=> s l9 and l10

L11 0 L9 AND L10

=> d l9 1

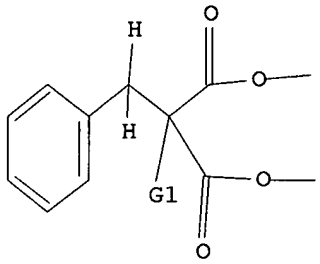
L9 ANSWER 1 OF 106 CA COPYRIGHT 1998 ACS
AN 127:358066 CA
TI Simple dissolution-reaction model for enzymic conversion of suspension of solid substrate
AU Wolff, A.; Zhu, L.; Kielland, V.; Straathof, A. J. J.; Jongejan, J. A.; Heijnen, J. J.
CS Department Biochemical Engineering, Delft University Technology, Delft, NL-2628 BC, Neth.
SO Biotechnol. Bioeng. (1997), 56(4), 433-440
CODEN: BIBIAU; ISSN: 0006-3592
PB Wiley
DT Journal
LA English

=> d 2-106 an ti

L11 HAS NO ANSWERS
'AN TI ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains data.
SDA ----- All Structure DAta (image, attributes, connection table and map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:
<------User Break------>

ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:.

L2 STR



G1 Me,Et,n-Pr

Structure attributes must be viewed using STN Express query preparation.
L5 SCR 1839
L8 128 SEA FILE=REGISTRY SSS FUL L2 NOT L5
L9 106 SEA FILE=CA L8
L10 1713 SEA FILE=CA ARYLPROPANOL? OR BENZENEPROPANOL? OR PHENYLPROPANOL?
L11 0 SEA FILE=CA L9 AND L10

=> d 19 2 hit

L9 ANSWER 2 OF 106 CA COPYRIGHT 1998 ACS
IT 77497-74-6P 79261-58-8P 79276-05-4P 80102-92-7P 99953-00-1P
189093-95-6P 189094-48-2P 194857-79-9P 194857-81-3P
194857-83-5P 194857-84-6P 194857-85-7P 194857-86-8P
194857-88-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of dimethyltyrosyl isoquinolinecarboxylate derivs. as .delta. opioid antagonists)

=> d 19 3-106 an hit

L9 ANSWER 3 OF 106 CA COPYRIGHT 1998 ACS
AN 126:301343 CA
IT **189287-72-7P** 189287-77-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 4 OF 106 CA COPYRIGHT 1998 ACS
AN 126:144291 CA
IT 588-96-5P, 1-Bromo-4-ethoxybenzene 874-31-7P, 2-Amino-5-chloro-3-methoxypyrazine 1006-63-9P 1458-03-3P 2156-04-9P, 4-Vinylphenylboronic acid 6684-06-6P, 2-Chloro-3-pyridinesulfonyl chloride 16152-51-5P, 4-Isopropylphenylboronic acid 17865-11-1P

22237-13-4P, 4-Ethoxyphenylboronic acid 33332-29-5P, 2-Amino-5-chloropyrazine 36603-49-3P, 2-(4-Bromophenoxy)-2H-tetrahydropyran 39969-56-7P, 1-Bromo-4-propoxybenzene 49660-93-7P, 1-(4-Bromophenyl)-2-methyl-1-propanone 63139-21-9P, 4-Ethylphenylboronic acid 66735-01-1P, 2-Methyl-3-(4-bromophenyl)propanoic acid **70146-85-9P**, Diethyl 2-(4-bromobenzyl)-2-methylmalonate 74290-65-6P, 2-Amino-3-bromo-5-methylpyrazine 76537-18-3P, 2-Amino-3-bromo-5-chloropyrazine 81183-58-6P 89464-87-9P, 2-Amino-3-methoxy-5-methylpyrazine 91011-76-6P, 4-(Diethylamino)phenylboronic acid 96833-41-9P, 5-Amino-2-chloro-4-methoxypyrimidine 99768-12-4P, 4-Methoxycarbonylphenylboronic acid 101251-09-6P, 4-Acetamidophenylboronic acid 123324-71-0P, 4-tert-Butylphenylboronic acid 134150-01-9P, 4-Propylphenylboronic acid 175885-77-5P, Dimethyl(3-pyridyl)borane 179251-28-6P
179251-29-7P 182281-01-2P 186497-45-0P 186497-46-1P
186497-47-2P 186497-48-3P 186497-49-4P 186497-50-7P
186497-51-8P 186497-52-9P 186497-53-0P, 4-Nitrophenyl 2-chloropyridine-3-sulfonate 186497-54-1P 186497-55-2P
186497-56-3P 186497-57-4P 186497-58-5P 186497-59-6P
186497-60-9P 186497-61-0P 186497-62-1P 186497-63-2P
186497-64-3P 186497-65-4P 186497-66-5P 186497-67-6P, 4-Propoxyphenylboronic acid 186497-68-7P 186497-69-8P
186497-70-1P 186497-71-2P 186497-72-3P, 2-Methyl-3-(4-bromophenyl)-1-propanol 186497-73-4P 186497-74-5P 186497-75-6P
186497-76-7P 186497-77-8P 186497-78-9P 186497-79-0P, 4-Allylphenylboronic acid 186497-80-3P 186497-81-4P
186497-82-5P 186497-83-6P 186497-84-7P, 4-(2-Methyl-2-propenyl)phenylboronic acid 186497-85-8P 186497-86-9P
186497-87-0P 186497-88-1P 186497-89-2P 186497-90-5P
186497-91-6P 186497-92-7P 186497-93-8P 186497-94-9P
186497-95-0P 186497-96-1P 186497-97-2P 186497-98-3P
186497-99-4P 186498-00-0P 186498-01-1P 186498-02-2P, 4-Morpholinophenylboronic acid 186498-03-3P 186498-04-4P
186498-05-5P 186498-06-6P 186498-07-7P 186498-08-8P
186498-09-9P, 1-(4-Bromophenoxy)-2-methyl-2-propanol 186498-10-2P
186498-11-3P 186498-12-4P, 1-(4-Bromophenoxy)-2-methyl-1-propanol
186498-13-5P 186498-14-6P 186498-15-7P 186498-16-8P
186498-17-9P 186498-18-0P 186498-19-1P 186498-20-4P
186498-21-5P 186498-22-6P 186498-23-7P, 2-(4-Bromophenyl)-2-propyl-1,3-dioxolane 186498-24-8P 186498-25-9P 186498-26-0P
186498-27-1P 186498-28-2P 186498-29-3P 186498-30-6P
186498-31-7P 186498-32-8P 186498-33-9P 186498-35-1P
186498-37-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of n-pyrazinyl-2-phenyl-3-pyridinesulfonamides and analogs endothelin receptor antagonists)

L9 ANSWER 5 OF 106 CA COPYRIGHT 1998 ACS
AN 125:248797 CA
IT 66191-99-9P 66192-08-3P **66192-12-9P** 66192-21-0P
93098-67-0P 102539-53-7P, 4-Bromo-3-methyl-1-indanone
112549-07-2P 174702-59-1P 174702-74-0P 174702-75-1P
174702-76-2P 175649-09-9P 182056-57-1P 182056-62-8P
182056-68-4P 182056-74-2P 182188-80-3P 182188-81-4P
182188-82-5P 182188-83-6P 182188-86-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation)
(intermediate in metallocene catalyst manuf.; aluminoxane-free catalyst for manuf. of polyolefins with good particle properties)

L9 ANSWER 6 OF 106 CA COPYRIGHT 1998 ACS
AN 125:248793 CA
IT **66192-12-9P** 149080-24-0P 174702-59-1P 182056-40-2P
182056-62-8DP, diastereomeric derivs. 182056-68-4P 182056-74-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction in manuf. of metallocene catalysts for polymn. of .alpha.-olefins)

L9 ANSWER 7 OF 106 CA COPYRIGHT 1998 ACS
AN 125:221062 CA

IT **55114-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; synthesis of benzylpropionic acid)

L9 ANSWER 8 OF 106 CA COPYRIGHT 1998 ACS
AN 124:9404 CA
IT 1009-67-2P 38385-67-0P **55114-30-2P** 118970-92-6P
118970-96-0P 127986-89-4P 171080-58-3P 171080-59-4P
171234-86-9P 171234-87-0P 171234-89-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(optically active aminoazirines in synthesis of
methylphenylalanine synthons and some model peptides)

L9 ANSWER 9 OF 106 CA COPYRIGHT 1998 ACS
AN 123:341302 CA
IT 452-63-1P, 2-Bromo-5-fluorotoluene 609-08-5P, Diethyl
methylmalonate 923-06-8P, 2-Bromosuccinic acid 7719-09-7P,
Thionyl chloride **170927-02-3P** 170927-03-4P
170927-04-5P 170927-05-6P 170927-06-7P 170927-07-8P
170927-08-9P 170927-09-0P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); USES (Uses)
(reaction in prepn. of halogenated bisphenylindenyl transition
metal complexes as polymn. catalysts)

L9 ANSWER 10 OF 106 CA COPYRIGHT 1998 ACS
AN 123:256359 CA
IT 585-50-2P, 3-(3-Trifluoromethylphenyl)propionic acid 53473-36-2P,
3-(4-Trifluoromethylphenyl)propionic acid 94022-99-8P,
3-(2-Trifluoromethylphenyl)propionic acid 168833-77-0P,
3-(3-Trifluoromethoxyphenyl)propionic acid **168833-78-1P**,
Diethyl 2-methyl-2-(3-trifluoromethylphenyl)malonate 168833-79-2P,
2-Methyl-3-(3-trifluoromethylphenyl)propionic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of (phenylalkanoyl)guanidines with perfluoroalkyl groups
as sodium-hydrogen antiporter inhibitors)

L9 ANSWER 11 OF 106 CA COPYRIGHT 1998 ACS
AN 123:188478 CA
IT 128-37-0, Ionol, biological studies 128-37-0D, Ionol, derivs.
616-55-7 67739-15-5 67739-21-3 132030-09-2 132030-10-5
132030-11-6 **132030-12-7** 132030-14-9 132030-15-0
132054-20-7 132054-21-8 132054-22-9 132054-23-0 167773-31-1
RL: BAC (Biological activity or effector, except adverse); THU
(Therapeutic use); BIOL (Biological study); USES (Uses)
(protective effects of lipo- and water-sol. ionol antioxidants on
liver cytochrome P 450 system during lipid peroxidn.)

L9 ANSWER 12 OF 106 CA COPYRIGHT 1998 ACS
AN 123:143767 CA
IT 18880-00-7P **162821-86-5P** 162821-88-7P 166375-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(asym. chemoenzymic synthesis of fenpropimorph)

L9 ANSWER 13 OF 106 CA COPYRIGHT 1998 ACS
AN 123:56334 CA
IT **131780-99-9P** 131781-62-9P 131781-63-0P 142909-98-6P
164225-02-9P 164225-03-0P 164225-04-1P 164225-05-2P
164225-09-6P 164225-10-9P 164575-84-2P 164575-85-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., properties, and receptor binding of both enantiomers of
DAU 5750)

L9 ANSWER 14 OF 106 CA COPYRIGHT 1998 ACS
AN 123:55499 CA
IT 351-54-2P, 3-Fluoro-4-methoxybenzaldehyde 1550-35-2P,
2,4-Difluorobenzaldehyde 5464-10-8P, 6-Methoxy-2-methylindanone
16204-11-8P 17304-68-6P 22138-69-8P, ..alpha..-Methyl-..beta..-
(p-methylthiophenyl) propionic acid 22138-72-3P,
p-Fluoro-.alpha.-methylcinnamic acid 22138-73-4P,

p-Fluoro-.alpha.-methylhydrocinnamic acid 27961-57-5P, Ethyl 2-hydroxy-2-(p-methoxyphenyl)-1-methylpropionate 32004-52-7P 32004-54-9P 32004-55-0P, 3,4-Difluoro-..alpha..-methylcinnamic acid 32004-56-1P 32004-57-2P, 5,6-Difluoro-2-methyl-1-indanone 32004-58-3P 32004-59-4P 32004-62-9P 32004-63-0P, 5-Fluoro-6-methoxy-2-methylindanone 32004-64-1P 32004-65-2P 32004-66-3P 32004-67-4P 32004-70-9P, 2,4-Difluoro-.alpha.-methylcinnamic acid 32004-71-0P 32004-72-1P, 4,6-Difluoro-2-methylindanone 32004-73-2P 32004-75-4P 32040-88-3P 33036-54-3P 34036-07-2P, 3,4-Difluorobenzaldehyde 37794-19-7P, 6-Fluoro-2-methylindanone 50703-56-5P 52427-11-9P, ..alpha..-Methyl-..beta..-(p-methoxyphenyl)propionic acid 99046-64-7P 142958-52-9P 142988-15-6P **144871-78-3P** 145900-54-5P 145900-55-6P 145900-59-0P 145928-09-2P 145928-10-5P 164394-18-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(use of substituted sulfonyl indenylacetic and -propionic acids and esters for treatment of precancerous lesions)

L9 ANSWER 15 OF 106 CA COPYRIGHT 1998 ACS
AN 123:9313 CA
IT 37699-43-7P 68707-69-7P **162821-86-5P** 163593-69-9P, 4-Methoxy-2,3-dimethylpyridine 163593-70-2P 163593-71-3P 163593-72-4P 163593-73-5P 163593-74-6P 163593-75-7P 163593-76-8P 163593-77-9P 163593-78-0P 163593-79-1P 163593-80-4P 163593-81-5P 163593-82-6P 163593-83-7P 163593-84-8P 163593-85-9P 163593-86-0P 163593-87-1P 163593-88-2P 163593-89-3P 163593-90-6P 163593-92-8P 163593-93-9P 163593-94-0P 163593-95-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of quinazolidineethanols as ergosterol aza analogs)

L9 ANSWER 16 OF 106 CA COPYRIGHT 1998 ACS
AN 122:289049 CA
IT **162821-86-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 17 OF 106 CA COPYRIGHT 1998 ACS
AN 122:31546 CA
IT 1009-67-2P 2437-08-3P 5669-16-9P 6149-41-3P 14367-54-5P 14367-67-0P 25177-85-9P 34917-00-5P **55114-30-2P** 81250-33-1P 81250-34-2P 85677-12-9P 98191-23-2P 102284-73-1P 102284-74-2P 123162-26-5P 130277-37-1P 130277-38-2P 130404-30-7P 130404-31-8P 137685-73-5P 137685-75-7P 137685-76-8P 137685-77-9P 137685-78-0P 137685-80-4P 137685-81-5P 137685-82-6P 137685-83-7P 137685-84-8P 137685-85-9P 137706-77-5P 159722-55-1P 159722-56-2P 159722-57-3P 159722-58-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of xanthine-deriv. adenosine A1 receptor antagonists)

L9 ANSWER 18 OF 106 CA COPYRIGHT 1998 ACS
AN 121:300564 CA
IT **159179-25-6** 159249-19-1 159249-20-4
RL: RCT (Reactant)
(failed; prepn. of optically active ketone by palladium-induced cascade reaction from racemic .beta.-keto ester)

L9 ANSWER 19 OF 106 CA COPYRIGHT 1998 ACS
AN 121:35028 CA
IT **155827-64-8P** 155827-65-9P 155827-66-0P 155827-67-1P 155827-68-2P 155827-69-3P 155827-70-6P 155827-71-7P 155827-72-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of pesticide)

L9 ANSWER 20 OF 106 CA COPYRIGHT 1998 ACS
AN 121:8791 CA
IT 4438-01-1P 13738-64-2P, 2-(Butoxymethyl)phenol 14680-18-3P

20920-83-6P, Phenol, 2-ethoxymethyl 33316-78-8P, Phenol, 2-(1-methylethoxy)methyl 65538-44-5P 146425-43-6P 151291-56-4P 155441-05-7P, 2-(2-Nitro-2-phenylethyl)phenol 155441-08-0P 155441-09-1P 155441-10-4P **155441-11-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, from [(benzotriazolyl)alkyl]phenol)

L9 ANSWER 21 OF 106 CA COPYRIGHT 1998 ACS
AN 120:244286 CA
IT 5217-04-9P 26673-29-0P 41975-67-1P **55114-30-2P**
91910-16-6P 137344-17-3P 138536-55-7P 138536-59-1P
138536-62-6P 138536-72-8P 154194-02-2P 154194-04-4P
154194-05-5P 154194-06-6P 154194-07-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 77320-46-8 134079-01-9 138536-54-6 **138536-56-8**
138536-57-9 138536-58-0 154194-00-0
RL: RCT (Reactant)
(reactant, in cyclization by stannyl anion generated from tributytrimethylsilylstannane and benzyltriethylammonium chloride)

L9 ANSWER 22 OF 106 CA COPYRIGHT 1998 ACS
AN 119:108172 CA
IT 94-21-3 106-92-3 495-76-1, 1,3-Benzodioxole-5-methanol
867-13-0 5465-67-8 15190-10-0 **77611-64-4**
RL: ANST (Analytical study)
(identification of large mol. fragment in, using IR spectra database)

L9 ANSWER 23 OF 106 CA COPYRIGHT 1998 ACS
AN 119:95001 CA
IT 112818-04-9 134079-01-9 **138536-56-8** 138536-57-9
147973-92-0
RL: RCT (Reactant)
(cyclization of, by stannyl anion generated from (trimethylsilyl)tributylstannane and fluoride ion)

L9 ANSWER 24 OF 106 CA COPYRIGHT 1998 ACS
AN 119:89821 CA
IT 1069-38-1 4358-88-7 14189-95-8 15399-27-6 16108-06-8
30697-69-9 62436-70-8 **95929-64-9** 149198-62-9
RL: RCT (Reactant)
(reaction of, with chymotrypsin, calcn. of enantioselectivity in)

L9 ANSWER 25 OF 106 CA COPYRIGHT 1998 ACS
AN 118:147318 CA
IT 4371-04-4P 7598-70-1P 19157-51-8P 110270-80-9P
135460-43-4P 135460-53-6P 135460-79-6P 135460-80-9P
144404-37-5P 144842-69-3P 144842-70-6P 144842-71-7P
144842-72-8P 144842-76-2P 144842-77-3P 144842-78-4P
144842-80-8P 144842-81-9P 144842-82-0P 144842-83-1P
144842-84-2P 144842-85-3P 144842-86-4P 144842-88-6P
144842-89-7P 144842-90-0P 144842-91-1P 144842-92-2P
144842-93-3P 144842-94-4P 144842-96-6P 144842-98-8P
144842-99-9P 144843-01-6P 144843-02-7P 144843-04-9P
144843-05-0P 144843-06-1P 144843-09-4P 144843-10-7P
144843-11-8P 144843-12-9P 144863-05-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of diagnostic and therapeutic chelants)

L9 ANSWER 26 OF 106 CA COPYRIGHT 1998 ACS
AN 118:147290 CA
IT 7598-70-1P 21626-93-7P 119822-20-7P 119822-21-8P
135460-43-4P 135460-44-5P 135460-45-6P 144404-12-6P
144404-13-7P 144404-15-9P 144404-16-0P 144404-18-2P
144404-20-6P 144404-21-7P 144404-22-8P 144404-23-9P
144404-25-1P 144404-26-2P 144404-27-3P 144404-28-4P
144404-29-5P 144404-30-8P 144404-31-9P 144404-32-0P

144404-33-1P 144404-34-2P 144404-35-3P 144404-37-5P
144404-38-6P 144404-39-7P 144404-40-0P 144404-42-2P
144943-47-5P 144943-48-6P 144943-49-7P 144943-51-1P
144943-52-2P 144943-53-3P 144943-54-4P 144962-60-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of diagnostic and therapeutic chelating agents)

L9 ANSWER 27 OF 106 CA COPYRIGHT 1998 ACS
AN 118:101720 CA
IT 22138-69-8P 81579-29-5P 123162-26-5P 123392-36-9P
133273-97-9P 133778-23-1P 144871-72-7P 144871-73-8P
144871-74-9P 144871-75-0P 144871-76-1P 144871-77-2P
144871-78-3P 144871-79-4P 144871-80-7P 144871-81-8P
144871-82-9P 144871-83-0P 144871-84-1P 144871-85-2P
144871-86-3P 144871-87-4P 144871-88-5P 144871-89-6P
144871-90-9P 144871-91-0P 144871-92-1P 144871-93-2P
144871-94-3P 144871-95-4P 144871-96-5P 144871-97-6P
144871-98-7P 144871-99-8P 144872-00-4P 144872-01-5P
144872-02-6P 144872-03-7P 144872-04-8P 144872-05-9P
144872-06-0P 144872-07-1P 144872-08-2P **144872-09-3P**
144872-10-6P 144872-11-7P 144872-12-8P 144872-13-9P
144872-14-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of adenosine receptor antagonists)

L9 ANSWER 28 OF 106 CA COPYRIGHT 1998 ACS
AN 118:101671 CA
IT 351-54-2P, 3-Fluoro-4-methoxybenzaldehyde 1550-35-2P,
2,4-Difluorobenzaldehyde 5464-10-8P, 6-Methoxy-2-methylindanone
16204-11-8P 17304-68-6P 22138-69-8P 22138-72-3P,
p-Fluoro-.alpha.-methylcinnamic acid 22138-73-4P,
p-Fluoro-.alpha.-methylhydrocinnamic acid 27961-57-5P
32004-52-7P 32004-54-9P 32004-55-0P 32004-56-1P 32004-57-2P
32004-58-3P 32004-59-4P 32004-62-9P 32004-63-0P 32004-64-1P
32004-65-2P 32004-66-3P 32004-67-4P 32004-68-5P 32004-70-9P
32004-71-0P 32004-72-1P 32004-73-2P 32004-75-4P 32040-88-3P
32165-56-3P 33036-54-3P 33036-55-4P 33036-56-5P 33036-57-6P
34036-07-2P, 3,4-Difluorobenzaldehyde 37794-19-7P,
6-Fluoro-2-methylindanone 38194-50-2P 50703-56-5P 99046-64-7P
142958-46-1P 142958-47-2P 142958-48-3P 142958-51-8P
142958-52-9P 142988-13-4P 142988-15-6P **144871-78-3P**
145900-48-7P 145900-49-8P 145900-50-1P 145900-51-2P
145900-52-3P 145900-53-4P 145900-54-5P 145900-55-6P
145900-56-7P 145900-57-8P 145900-58-9P 145900-59-0P
145900-60-3P 145900-61-4P 145928-08-1P 145928-09-2P
145928-10-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for anticancer agent)

L9 ANSWER 29 OF 106 CA COPYRIGHT 1998 ACS
AN 117:233535 CA
IT 52252-58-1P 144344-86-5P 144344-87-6P 144344-88-7P
144344-89-8P **144344-90-1P** 144344-91-2P 144344-92-3P
144344-93-4P 144344-94-5P 144344-95-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 30 OF 106 CA COPYRIGHT 1998 ACS
AN 117:7850 CA
IT **141352-95-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acid hydrolysis-decarboxylation of)

L9 ANSWER 31 OF 106 CA COPYRIGHT 1998 ACS
AN 116:83341 CA
IT **138089-93-7P 138089-94-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 32 OF 106 CA COPYRIGHT 1998 ACS
AN 116:83317 CA
IT **118688-45-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 33 OF 106 CA COPYRIGHT 1998 ACS
AN 116:79776 CA
IT **95929-64-9**
RL: RCT (Reactant)
(transesterification of, stereoselective, with benzyl alc. in org. solvents, enzyme-catalyzed)

L9 ANSWER 34 OF 106 CA COPYRIGHT 1998 ACS
AN 116:58915 CA
IT 5217-04-9P 26673-29-0P 41975-67-1P **55114-30-2P**
63831-51-6P 67714-28-7P 91910-16-6P 137344-17-3P
138536-48-8P 138536-49-9P 138536-51-3P 138536-52-4P
138536-53-5P 138536-55-7P 138536-60-4P 138536-61-5P
138536-62-6P 138536-64-8P 138536-65-9P 138536-67-1P
138536-68-2P 138536-69-3P 138536-70-6P 138536-71-7P
138536-72-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 99-49-0 930-68-7, 2-Cyclohexen-1-one 112818-04-9 134079-00-8
134079-01-9 137344-19-5 138536-50-2 138536-54-6
138536-56-8 138536-57-9 138536-58-0 138536-59-1
138536-63-7 138536-66-0
RL: RCT (Reactant)
(reaction of, with stannyl anion generated from tributyl(trimethylsilyl)stannane in presence of quaternary ammonium halides)

L9 ANSWER 35 OF 106 CA COPYRIGHT 1998 ACS
AN 116:6578 CA
IT 1009-67-2P 2437-08-3P 5669-16-9P 6149-41-3P 14367-54-5P
14367-67-0P 25177-85-9P 34917-00-5P **55114-30-2P**
81250-33-1P, 1,3-Dipropyl-5-nitroso-6-aminouracil 81250-34-2P
85677-12-9P 98191-23-2P 102284-73-1P 102284-74-2P
128544-04-7P 130277-37-1P 130277-38-2P 130404-30-7P
130404-31-8P 137685-73-5P 137685-74-6P 137685-75-7P
137685-76-8P 137685-77-9P 137685-78-0P 137685-79-1P
137685-80-4P 137685-81-5P 137685-82-6P 137685-83-7P
137685-84-8P 137685-85-9P 137706-77-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for selective adenosine receptor agent)

L9 ANSWER 36 OF 106 CA COPYRIGHT 1998 ACS
AN 115:255826 CA
IT 4371-04-4P 7598-70-1P 10255-94-4P 53651-72-2P 119822-20-7P
119822-21-8P **135460-43-4P** 135460-44-5P 135460-45-6P
135460-46-7P 135460-47-8P 135460-48-9P 135460-49-0P
135460-50-3P 135460-51-4P 135460-52-5P 135460-53-6P
135460-54-7P 135460-55-8P 135460-56-9P 135460-57-0P
135460-58-1P 135460-59-2P 135460-60-5P 135460-61-6P
135460-62-7P 135460-63-8P 135460-64-9P 135460-65-0P
135460-66-1P 135460-67-2P 135460-68-3P 135460-69-4P
135460-70-7P 135460-71-8P 135460-72-9P 135460-73-0P
135460-74-1P 135460-75-2P 135460-76-3P 135460-77-4P
135460-78-5P 135460-79-6P 135460-80-9P 135460-81-0P
135460-82-1P 135460-83-2P 135460-84-3P 135460-85-4P
135460-86-5P 135460-87-6P 135460-88-7P 135460-89-8P
135460-90-1P 135460-91-2P 135484-16-1P 135484-41-2P
135484-42-3P 135484-43-4P 135546-86-0P 137164-59-1P
137164-60-4P 137164-61-5P 138339-82-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of ligands and radioactive isotope complexes)

L9 ANSWER 37 OF 106 CA COPYRIGHT 1998 ACS
AN 115:114819 CA
IT **132629-17-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., hydrolysis, and decarboxylation of)

L9 ANSWER 38 OF 106 CA COPYRIGHT 1998 ACS
AN 114:159616 CA
IT **95929-64-9** 102508-03-2
RL: BIOL (Biological study)
(carboxylesterase isoenzymes of liver enantiotopic selectivity for, DMSO effect on)

L9 ANSWER 39 OF 106 CA COPYRIGHT 1998 ACS
AN 114:123020 CA
IT **132629-17-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymic hydrolysis of, with esterase)
IT **132629-16-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and selective enzymic hydrolysis of, with esterase, stereochem. of)

L9 ANSWER 40 OF 106 CA COPYRIGHT 1998 ACS
AN 114:81865 CA
IT 59803-35-9P 131780-91-1P 131780-92-2P, 5-Fluoro-2-nitrobenzylamine 131780-93-3P, 5-Carbamoyl-2-nitrobenzylamine 131780-94-4P, 2-Hydroxy-6-nitrobenzylamine hydrochloride 131780-95-5P, 2-Methyl-6-nitrobenzylamine 131780-96-6P, 2-Methyl-3-nitrobenzylamine 131780-97-7P, 4-Fluoro-2-nitrobenzylamine 131780-98-8P **131780-99-9P**
131781-00-5P 131781-01-6P 131781-02-7P 131781-03-8P
131781-04-9P 131781-05-0P 131781-06-1P 131781-07-2P
131781-08-3P 131781-09-4P 131781-10-7P 131781-11-8P
131781-12-9P 131781-13-0P 131781-14-1P 131781-15-2P
131781-16-3P 131781-17-4P 131781-18-5P 131781-19-6P
131781-20-9P 131781-21-0P 131781-22-1P 131781-23-2P
131781-24-3P 131781-25-4P 131781-26-5P 131781-27-6P
131781-28-7P 131781-29-8P 131781-30-1P 131781-31-2P
131781-32-3P 131781-33-4P 131781-34-5P 131781-35-6P
131781-36-7P 131781-37-8P 131781-38-9P 131781-39-0P
131781-40-3P 131781-41-4P 131781-42-5P 131781-43-6P
131781-44-7P 131781-45-8P 131781-46-9P 131781-47-0P
131781-48-1P 131781-49-2P 131781-50-5P 131781-51-6P
131781-52-7P 131781-53-8P 131781-54-9P 131781-55-0P
131781-56-1P 131781-57-2P 131781-58-3P 131781-59-4P
131781-60-7P 131781-61-8P 131781-62-9P 131781-63-0P
131799-59-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of antimuscarinic agent)

L9 ANSWER 41 OF 106 CA COPYRIGHT 1998 ACS
AN 114:74727 CA
IT 1020-31-1 67739-15-5 67739-21-3 132030-09-2 132030-10-5 132030-11-6 **132030-12-7** 132030-13-8 132030-14-9
132030-15-0 132054-20-7 132054-21-8 132054-22-9 132054-23-0
RL: PRP (Properties)
(antioxidant effects of, in biol. membranes, structure in relation to)

L9 ANSWER 42 OF 106 CA COPYRIGHT 1998 ACS
AN 114:74726 CA
IT 1020-31-1 67739-15-5 67739-21-3 132030-09-2 132030-10-5 132030-11-6 **132030-12-7** 132030-13-8 132030-14-9
132030-15-0 132054-20-7 132054-21-8 132054-22-9 132054-23-0
RL: PRP (Properties)
(antioxidant effects of, structure in relation to)

L9 ANSWER 43 OF 106 CA COPYRIGHT 1998 ACS

AN 113:171992 CA
IT **21118-89-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and bromination of)

L9 ANSWER 44 OF 106 CA COPYRIGHT 1998 ACS
AN 112:216849 CA
IT 76-67-5, Diethyl ethylphenylmalonate 76-72-2 93-58-3, Methylbenzoate 99-75-2, Methyl-p-toluate 121-98-2, Methyl-p-anisate 3195-24-2, Diethyl diallylmalonate **76154-00-2**
RL: RCT (Reactant)
(electrochem. reaction of, with urea)

L9 ANSWER 45 OF 106 CA COPYRIGHT 1998 ACS
AN 112:179015 CA
IT 76-67-5 76-72-2 77-25-8 3195-24-2 **76154-00-2**
RL: RCT (Reactant)
(electrochem. reaction of, with urea, barbituric acid from)

L9 ANSWER 46 OF 106 CA COPYRIGHT 1998 ACS
AN 112:21367 CA
IT 597-55-7P 607-81-8P **55114-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)

L9 ANSWER 47 OF 106 CA COPYRIGHT 1998 ACS
AN 112:20729 CA
IT 3526-45-2P 4895-96-9P 4992-02-3P 5355-17-9P, 4-(Methoxymethyl)phenol 5635-98-3P, 2-(Methoxymethyl)phenol 15451-07-7P 24619-86-1P 33033-90-8P, 4-(Anilinomethyl)phenol 45966-19-6P 54373-27-2P 55116-30-8P, 2-(Azidomethyl)phenol 55116-31-9P, 4-(Azidomethyl)phenol 66287-29-4P 77094-90-7P 92196-19-5P 112621-26-8P 112621-27-9P 120677-37-4P 124389-46-4P 124389-47-5P 124389-50-0P 124389-51-1P 124389-52-2P, 4-Hydroxycinnamyl azide 124389-53-3P **124389-54-4P** 124389-55-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 48 OF 106 CA COPYRIGHT 1998 ACS
AN 111:39187 CA
IT 121482-58-4P **121482-62-0P** 121482-65-3P 121482-70-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation of, with tetrahydrophthalic anhydride, in prepn. of herbicide)
IT 55417-40-8P **121482-60-8P** 121482-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and nitration of, in prepn. of herbicide)
IT 121482-57-3P **121482-61-9P** 121482-64-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of, in prepn. of herbicide)

L9 ANSWER 49 OF 106 CA COPYRIGHT 1998 ACS
AN 111:7047 CA
IT **52086-50-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 50 OF 106 CA COPYRIGHT 1998 ACS
AN 110:210971 CA
IT 21186-54-9P 99531-07-4P **120681-58-5P**
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manuf. of, from corresponding diester, by enzymic resoln.)

L9 ANSWER 51 OF 106 CA COPYRIGHT 1998 ACS
AN 110:153913 CA
IT **118688-44-1P 118688-45-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and hydrogenation of)
IT **118688-46-3P 118688-47-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon.-decarboxylation of)

L9 ANSWER 52 OF 106 CA COPYRIGHT 1998 ACS
AN 110:82286 CA
IT **94430-87-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 53 OF 106 CA COPYRIGHT 1998 ACS
AN 108:146043 CA
IT **113741-14-3**
RL: BIOL (Biological study)
(chymotrypsin interaction with)
IT 49769-78-0 **95929-64-9**
RL: RCT (Reactant)
(hydrolysis of, by chymotrypsin, kinetics of, enzyme substrate specificity and stereoselectivity prediction in relation to)
IT 607-81-8 **5846-22-0 21118-89-8 55114-30-2**
RL: RCT (Reactant)
(hydrolysis of, by chymotrypsin, product chirality in)

L9 ANSWER 54 OF 106 CA COPYRIGHT 1998 ACS
AN 108:5839 CA
IT 76-72-2P 77-25-8P 103-29-7P 580-35-8P, 2,4,6-Triphenylpyridine
2049-66-3P 6731-58-4P 71501-13-8P 73062-47-2P 73086-80-3P
73286-97-2P **76154-00-2P** 107449-78-5P 111784-48-6P
111784-49-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 55 OF 106 CA COPYRIGHT 1998 ACS
AN 106:192586 CA
IT 67-52-7DP, Barbituric acid, trimethoxybenzyl derivs. 50846-63-4P
50846-64-5P 50846-65-6P 50846-66-7P 50846-67-8P 50846-68-9P
50846-70-3P **50846-72-5P** 50846-73-6P 50846-75-8P
50846-76-9P 51031-82-4P **51031-83-5P** 51031-84-6P
56543-92-1P 56543-93-2P 56543-94-3P 56543-95-4P 56543-96-5P
56543-97-6P 56543-98-7P 56543-99-8P 56544-00-4P 56544-01-5P
56544-03-7P 56596-63-5P 56596-64-6P 57882-23-2P
77611-64-4P 108097-05-8P 108097-06-9P 108097-07-0P
108097-08-1P 108097-09-2P 108097-10-5P 108097-11-6P
108097-12-7P 108097-13-8P 108097-14-9P 108097-15-0P
108097-16-1P 108097-17-2P 108097-18-3P 108097-19-4P
108097-20-7P 108097-21-8P 108097-22-9P 108097-23-0P
108097-24-1P 108097-25-2P 108097-26-3P 108097-27-4P
108097-28-5P 108097-29-6P 108097-30-9P 108097-31-0P
108097-32-1P 108097-33-2P 108097-34-3P 108097-35-4P
108097-36-5P 108097-37-6P 108118-29-2P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antibacterial activity of, structure in relation to)

L9 ANSWER 56 OF 106 CA COPYRIGHT 1998 ACS
AN 106:119189 CA
IT 77738-20-6P 98506-66-2P 98506-67-3P 98514-81-9P 103633-30-3P
106419-73-2P 106419-74-3P **106419-75-4P** 106419-76-5P
106419-77-6P 106419-78-7P 106419-79-8P 106419-80-1P
106419-81-2P 106419-82-3P 106419-83-4P 106419-84-5P
106419-85-6P 106419-86-7P 106419-87-8P 106419-88-9P
106419-89-0P 106419-90-3P 106419-91-4P 106419-92-5P
106419-93-6P 106419-94-7P 106419-95-8P 106419-96-9P
106419-97-0P 106420-00-2P 106420-01-3P 106420-02-4P
106420-03-5P 106434-36-0P 106434-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to chromogenic crown ether)

L9 ANSWER 57 OF 106 CA COPYRIGHT 1998 ACS

AN 106:84121 CA
IT **105372-24-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

L9 ANSWER 58 OF 106 CA COPYRIGHT 1998 ACS
AN 106:32509 CA
IT **73120-65-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 59 OF 106 CA COPYRIGHT 1998 ACS
AN 105:208909 CA
IT **85301-63-9P** 85301-64-0P 85308-20-9P 85308-21-0P
85308-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation of, with guanidine)

L9 ANSWER 60 OF 106 CA COPYRIGHT 1998 ACS
AN 105:132945 CA
IT **104390-75-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)

L9 ANSWER 61 OF 106 CA COPYRIGHT 1998 ACS
AN 105:93463 CA
IT 108-59-8D, dialkylated 2917-78-4 **5846-22-0**
21118-89-8 95929-64-9 98061-06-4
RL: RCT (Reactant)
(reaction of, with carboxylesterase of liver, enantioselectivity
in, DMSO effect on)

L9 ANSWER 62 OF 106 CA COPYRIGHT 1998 ACS
AN 104:17316 CA
IT **5846-22-0P 21118-89-8P 95929-64-9P**
RL: PREP (Preparation)
(prepn. and hydrolysis by chymotrypsin plus esterase)

L9 ANSWER 63 OF 106 CA COPYRIGHT 1998 ACS
AN 103:123192 CA
IT 15326-95-1P 15326-96-2P 15374-23-9P 42361-33-1P
98190-97-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 64 OF 106 CA COPYRIGHT 1998 ACS
AN 103:122638 CA
IT 2049-70-9 2917-78-4 55114-29-9 **55114-30-2** 55898-43-6
65896-61-9 88253-94-5 98061-04-2 98061-05-3 98061-06-4
98061-07-5 98061-08-6
RL: RCT (Reactant)
(enzyme-catalyzed hydrolysis of)
IT **95929-64-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzyme-catalyzed hydrolysis of)

L9 ANSWER 65 OF 106 CA COPYRIGHT 1998 ACS
AN 102:166308 CA
IT 95929-63-8P **95929-64-9P** 95929-65-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by methoxycarbonylation-methylation of ester)

L9 ANSWER 66 OF 106 CA COPYRIGHT 1998 ACS
AN 100:121376 CA
IT **52528-74-2P 52528-76-4P 52528-77-5P**
89042-94-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for pterosin-E)

L9 ANSWER 67 OF 106 CA COPYRIGHT 1998 ACS

AN 99:211872 CA
IT **87482-89-1**
RL: RCT (Reactant)
(sapon. of)

L9 ANSWER 68 OF 106 CA COPYRIGHT 1998 ACS
AN 99:4853 CA
IT 38896-01-4P 86096-96-0P **86096-97-1P** 86096-98-2P
86097-00-9P 86097-01-0P 86097-02-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 69 OF 106 CA COPYRIGHT 1998 ACS
AN 98:160669 CA
IT **85301-63-9P** 85301-64-0P 85308-20-9P 85308-21-0P
85308-22-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation with guanidine)

L9 ANSWER 70 OF 106 CA COPYRIGHT 1998 ACS
AN 98:98679 CA
IT **55114-30-2P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in photolysis of [bis(ethoxycarbonyl)propyl]cobaloxime)

L9 ANSWER 71 OF 106 CA COPYRIGHT 1998 ACS
AN 98:13857 CA
IT **53979-20-7**
RL: RCT (Reactant)
(hydrolysis of, asym., with pig liver esterase, methyldopa synthesis in relation to)

L9 ANSWER 72 OF 106 CA COPYRIGHT 1998 ACS
AN 96:217479 CA
IT **80790-79-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 73 OF 106 CA COPYRIGHT 1998 ACS
AN 96:85262 CA
IT **80790-79-0**
RL: PROC (Process)
(conversion of, to (chlorohydroxyphenyl)methylpropanoate ester)

L9 ANSWER 74 OF 106 CA COPYRIGHT 1998 ACS
AN 95:6875 CA
IT **61227-49-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 75 OF 106 CA COPYRIGHT 1998 ACS
AN 94:29723 CA
IT 580-35-8P 6125-24-2P 34405-43-1P **76154-00-2P**
76154-01-3P 76154-02-4P 76154-03-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 76 OF 106 CA COPYRIGHT 1998 ACS
AN 93:95235 CA
IT **55114-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation of, with urea)

L9 ANSWER 77 OF 106 CA COPYRIGHT 1998 ACS
AN 92:215009 CA
IT 607-81-8P 609-08-5P 619-68-1P 831-91-4P 6731-58-4P
55114-30-2P 73062-47-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 78 OF 106 CA COPYRIGHT 1998 ACS
AN 92:146387 CA
IT 6619-58-5P 37765-73-4P 70146-77-9P **70146-83-7P**
73120-66-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
IT **73120-65-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 79 OF 106 CA COPYRIGHT 1998 ACS
AN 90:179912 CA
IT **70146-83-7P 70146-84-8P 70146-85-9P**
70146-86-0P 70146-87-1P 70146-88-2P
70146-89-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 80 OF 106 CA COPYRIGHT 1998 ACS
AN 88:152456 CA
IT **66192-10-7P** 66192-11-8P **66192-12-9P**
66192-13-0P 66192-14-1P 66192-15-2P **66192-16-3P**
66192-17-4P 66192-18-5P **66192-19-6P 66192-20-9P**
66192-21-0P 66192-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 81 OF 106 CA COPYRIGHT 1998 ACS
AN 87:135246 CA
IT **34928-28-4 34928-31-9 34928-35-3**
53979-21-8 53979-23-0 53979-25-2 **55114-30-2**
57737-37-8 **57737-40-3** 57737-41-4
RL: RCT (Reactant)
(cyclocondensation of, with benzoylurea)

L9 ANSWER 82 OF 106 CA COPYRIGHT 1998 ACS
AN 87:68521 CA
IT **16123-38-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 83 OF 106 CA COPYRIGHT 1998 ACS
AN 86:16505 CA
IT 16123-39-0P **61227-49-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)
IT **16123-38-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

L9 ANSWER 84 OF 106 CA COPYRIGHT 1998 ACS
AN 85:159759 CA
IT 60726-40-1 **60726-42-3**
RL: RCT (Reactant)
(hydrolysis and decarboxylation of)

L9 ANSWER 85 OF 106 CA COPYRIGHT 1998 ACS
AN 85:123658 CA
IT **60423-90-7P** 60424-11-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

L9 ANSWER 86 OF 106 CA COPYRIGHT 1998 ACS
AN 84:30997 CA
IT **57737-33-4 57737-34-5 57737-35-6**
57737-36-7 57737-37-8 **57737-38-9 57737-39-0**
57737-40-3 57737-41-4 **57749-46-9**
57749-47-0 57827-47-1
RL: RCT (Reactant)

(reaction of, with urea and phenylurea)

L9 ANSWER 87 OF 106 CA COPYRIGHT 1998 ACS
AN 83:205954 CA
IT 57373-96-3P **57373-97-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

L9 ANSWER 88 OF 106 CA COPYRIGHT 1998 ACS
AN 82:125326 CA
IT 83-13-6 133-13-1 596-75-8 607-81-8 1619-62-1 2163-44-2
2163-48-6 6065-59-4 34009-61-5 55114-29-9 **55114-30-2**
RL: RCT (Reactant)
(condensation of, with hydrazino-1-methyl-3-phenyl-1H-1,2,4-triazole)

L9 ANSWER 89 OF 106 CA COPYRIGHT 1998 ACS
AN 82:58420 CA
IT **53413-48-2P** 53413-49-3P 53413-50-6P **53413-51-7P**
53413-52-8P 53413-54-0P **53417-22-4P** 53417-23-5P
53417-25-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 90 OF 106 CA COPYRIGHT 1998 ACS
AN 82:57721 CA
IT 7402-30-4 **50846-71-4 50846-72-5** 50846-73-6
50846-74-7 50846-75-8 50846-76-9 **51031-83-5**
52478-15-6
RL: RCT (Reactant)
(cyclization of, with urea)

L9 ANSWER 91 OF 106 CA COPYRIGHT 1998 ACS
AN 81:152082 CA
IT 53979-19-4P **53979-20-7P 53979-21-8P**
53979-22-9P 53979-23-0P 53979-24-1P 53979-25-2P
53979-26-3P 53979-27-4P 53979-28-5P
53979-29-6P 53979-30-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis-decarboxylation of)

L9 ANSWER 92 OF 106 CA COPYRIGHT 1998 ACS
AN 80:145877 CA
IT 6619-57-4P **52086-50-7P** 52086-51-8P 52086-52-9P
52086-53-0P 52086-54-1P 52086-55-2P 52086-56-3P 52086-57-4P
52086-58-5P 52086-59-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 93 OF 106 CA COPYRIGHT 1998 ACS
AN 80:121128 CA
IT **52528-74-2P** 52528-75-3P **52528-76-4P**
52528-77-5P 52528-78-6P 52528-79-7P **52528-80-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 94 OF 106 CA COPYRIGHT 1998 ACS
AN 80:108570 CA
IT 7402-30-4 **50846-71-4 50846-72-5** 50846-73-6
50846-74-7 50846-75-8 50846-76-9 **51031-83-5**
52478-15-6
RL: RCT (Reactant)
(cyclization of, with urea)

L9 ANSWER 95 OF 106 CA COPYRIGHT 1998 ACS
AN 80:14957 CA
IT 7402-30-4 **50846-71-4 50846-72-5** 50846-73-6
50846-74-7 50846-75-8 50846-76-9 **51031-83-5**
51031-84-6
RL: RCT (Reactant)

(reaction of, with urea)

L9 ANSWER 96 OF 106 CA COPYRIGHT 1998 ACS
AN 76:34193 CA
IT **34928-23-9P 34928-24-0P 34928-25-1P**
34928-26-2P **34928-27-3P 34928-28-4P**
34928-29-5P 34928-30-8P **34928-31-9P**
34928-32-0P 34928-33-1P **34928-34-2P**
34928-35-3P 34928-36-4P 34928-37-5P 34928-38-6P
34928-39-7P 34928-40-0P 34928-41-1P 34928-42-2P 34928-43-3P
34928-44-4P 34928-45-5P 34928-46-6P 34928-47-7P 34928-48-8P
34928-49-9P 34928-50-2P 34928-51-3P **34939-47-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 97 OF 106 CA COPYRIGHT 1998 ACS
AN 73:56809 CA
IT 23578-06-5 26872-59-3 28499-98-1 29134-78-9 29134-79-0
29134-80-3 **29134-81-4** 29134-82-5 **29134-83-6**
29134-84-7 29134-86-9 29134-87-0 29260-09-1 29260-10-4
29431-16-1
RL: USES (Uses)
(antioxidants, for plastics)

L9 ANSWER 98 OF 106 CA COPYRIGHT 1998 ACS
AN 71:102006 CA
IT **5075-55-8P** 5075-58-1P 5075-66-1P 5120-54-7P
5120-57-0P 17875-53-5P 17945-43-6P 23858-68-6P 23858-75-5P
23858-76-6P 23858-77-7P 23858-78-8P 23858-79-9P 23858-80-2P
23858-81-3P 23858-82-4P 23858-83-5P 23858-84-6P 23858-85-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 99 OF 106 CA COPYRIGHT 1998 ACS
AN 71:91132 CA
IT 18595-14-7P 24078-21-5P 24078-23-7P 24078-24-8P 24078-25-9P
24078-26-0P 24078-27-1P **24078-28-2P** 24078-29-3P
24078-30-6P 24078-31-7P 24078-32-8P 24078-33-9P 24078-34-0P
24106-09-0P 24106-10-3P 24231-93-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 100 OF 106 CA COPYRIGHT 1998 ACS
AN 71:22328 CA
IT 16817-48-4P 16855-15-5P 16882-23-8P **23354-66-7P**
23364-97-8P 23365-24-4P 23365-25-5P 23365-26-6P 23365-27-7P
23365-28-8P 23365-29-9P 23365-30-2P 23365-31-3P 23365-32-4P
23365-33-5P 23365-34-6P 23365-35-7P 23413-10-7P 23413-11-8P
23421-65-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 101 OF 106 CA COPYRIGHT 1998 ACS
AN 70:87356 CA
IT 4478-10-8P 4982-31-4P 5743-02-2P 22291-52-7P
22291-53-8P 22291-54-9P 22291-55-0P 22291-56-1P
22291-57-2P 22291-58-3P 22291-59-4P 22291-60-7P 22359-78-0P
24876-54-8P 24876-55-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 102 OF 106 CA COPYRIGHT 1998 ACS
AN 70:47872 CA
IT 672-87-7P 824-94-2P **21118-89-8P** 21118-91-2P
21186-54-9P 22620-02-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 103 OF 106 CA COPYRIGHT 1998 ACS
AN 68:79003 CA

IT 16545-53-2 19988-88-6 20297-75-0 20297-76-1 20297-77-2
20297-78-3 20297-79-4 20297-80-7 20297-82-9 20297-84-1
20297-85-2 20297-86-3 20297-87-4 20297-88-5 20297-89-6
20297-90-9 20297-91-0 20297-92-1 20297-93-2 20297-94-3
20297-95-4 20370-18-7 20370-19-8 20370-20-1
20370-21-2
RL: USES (Uses)
(stabilizers (thermal), for propene polymers)

L9 ANSWER 104 OF 106 CA COPYRIGHT 1998 ACS
AN 68:29468 CA
IT 613-26-3P 782-23-0P 785-00-2P 2960-97-6P 3837-38-5P
14343-91-0P 15254-25-8P 17526-42-0P 17526-43-1P 17526-44-2P
17526-45-3P 17526-46-4P 17526-47-5P 17526-49-7P 17526-50-0P
17526-51-1P 17526-52-2P 17526-53-3P 17526-54-4P
17526-55-5P 17526-56-6P 17526-57-7P 17538-44-2P
17538-45-3P 17538-46-4P 17538-48-6P 17538-49-7P 17538-50-0P
17538-51-1P 17538-52-2P 17538-53-3P 17538-54-4P 17538-55-5P
17538-56-6P 17538-57-7P 17538-58-8P 17538-59-9P 17538-61-3P
17538-63-5P 17748-92-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

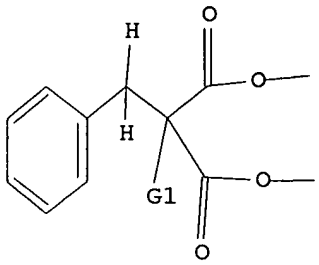
L9 ANSWER 105 OF 106 CA COPYRIGHT 1998 ACS
AN 67:100331 CA
IT 2445-28-5P 16123-36-7P 16123-37-8P **16123-38-9P**
16123-39-0P 16123-40-3P 16123-41-4P 16123-42-5P 16123-43-6P
16123-44-7P 16123-45-8P 16123-46-9P 16123-47-0P 16123-48-1P
16123-49-2P 16123-50-5P 16123-51-6P 16123-52-7P 16123-53-8P
16123-54-9P 16123-55-0P 16123-56-1P 16123-57-2P 16123-58-3P
16123-59-4P 16123-60-7P 16123-61-8P 16123-62-9P 16123-63-0P
16136-96-2P 16136-97-3P 16136-98-4P 16136-99-5P 16137-00-1P
16137-01-2P 16137-02-3P 16137-03-4P 16137-04-5P 16137-05-6P
16137-06-7P 16137-07-8P 16137-08-9P 16137-09-0P 16137-10-3P
16137-11-4P 16137-12-5P 16137-14-7P 16137-15-8P 16137-16-9P
16137-17-0P 16137-18-1P 16137-19-2P 16137-20-5P 16137-21-6P
16137-22-7P 16137-23-8P 16137-24-9P 16137-25-0P 16137-26-1P
16259-09-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 106 OF 106 CA COPYRIGHT 1998 ACS
AN 66:10834 CA
IT 13604-75-6P 13604-76-7P 13604-77-8P 13604-78-9P 13605-71-5P
13605-72-6P 13605-73-7P 13605-74-8P 13605-75-9P 13605-76-0P
13605-77-1P 13605-79-3P 13605-80-6P 13605-81-7P 13605-83-9P
13608-07-6P 13608-08-7P 13608-09-8P 13695-05-1P 14061-67-7P
14553-89-0P 14553-90-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

=> d 30-31 all

L11 HAS NO ANSWERS
'ALL ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains data.
SDA ----- All Structure DAta (image, attributes, connection table and map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:.

L2 STR



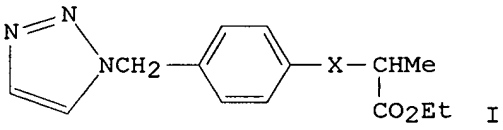
G1 Me,Et,n-Pr

Structure attributes must be viewed using STN Express query preparation.

```
L5              SCR 1839
L8          128 SEA FILE=REGISTRY SSS FUL L2 NOT L5
L9          106 SEA FILE=CA L8
L10        1713 SEA FILE=CA ARYLPROPANOL? OR BENZENEPROPANOL? OR PHENYLPR
                OPANOL?
L11           0 SEA FILE=CA L9 AND L10
```

=> d l9 30-31 all

L9 ANSWER 30 OF 106 CA COPYRIGHT 1998 ACS
AN 117:7850 CA
TI An 1,2,3-triazole derivative bioisoster of a potent in vitro prostaglandin synthesis inhibitor: preparation and biological activity
AU Biagi, Giuliana; Dell'omodarme, Giuliana; Giorgi, Irene; Livi, Oreste; Scartoni, Valerio
CS Ist. Chim. Farm. Tossicol., Univ. Pisa, Pisa, 56100, Italy
SO Farmaco (1992), 47(1), 91-8
CODEN: FRMCE8
DT Journal
LA English
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 2
GI



I

AB The prepn. of the triazole ester I (X = CH2), a methylenic bioisoster of an oxygenated compd. I (X = O), effective inhibitor of the prostaglandin synthesis in vitro is reported. Biol. evaluation of I (X = CH2) and of the corresponding acid shows that the compds. maintain a good enzymic inhibitory activity compared with indomethacin and aspirin.

ST ethoxycarbonylpropylbenzylimidazole prepn prostaglandin synthesis inhibitor; antiinflammatory ethoxycarbonylpropylbenzylimidazole; prostaglandin synthesis inhibitor bioisoster triazole

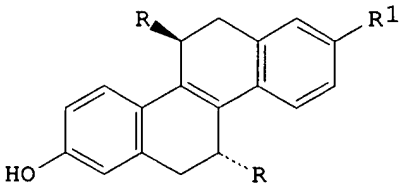
IT Inflammation inhibitors
(ethoxycarbonylpropylbenzylimidazoles)

IT Prostaglandins
RL: RCT (Reactant)
(inhibition of synthesis of, by ethoxycarbonylpropylbenzylimidazoles)

IT 100-14-1, p-Nitrobenzyl chloride
RL: RCT (Reactant)
(alkylation by, of di-Et methylmalonate)

IT 609-08-5, Diethyl methylmalonate
RL: RCT (Reactant)
(nitrobenzylation of)
IT **141352-95-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acid hydrolysis-decarboxylation of)
IT 141352-97-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acidation of)
IT 141353-00-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antiinflammatory activity of)
IT 52787-39-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and borohydride redn. of)
IT 141352-98-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of, with vinyl acetate, triazole deriv.)
IT 141352-96-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of, with hydrochloric acid)
IT 60423-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and formylation of)
IT 66735-03-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)
IT 103096-03-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sequential diazotization and cyanation of)
IT 141353-01-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 141352-99-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., esterification with ethanol and antiinflammatory activity of)

L9 ANSWER 31 OF 106 CA COPYRIGHT 1998 ACS
AN 116:83341 CA
TI 5,6,11,12-Tetrahydrochrysenes: synthesis of rigid stilbene systems designed to be fluorescent ligands for the estrogen receptor
AU Hwang, Kwang Jin; O'Neil, James P.; Katzenellenbogen, John A.
CS Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
SO J. Org. Chem. (1992), 57(4), 1262-71
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 25-28 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 9, 32
OS CJACS-IMAGE; CJACS
GI



I

AB A series of tetrahydrochrysenes, e.g. I (R = H, Me, Et, Pr, R1 = OH; R = Et, R1 = Ac, CO2Me, CN, CONH2, NO2), were prepd. as fluorescent ligands for the estrogen receptor. The stilbene chromophore in this tetracyclic system is held rigid and contains an electron-donating hydroxyl group at C-8, which corresponds to the phenolic hydroxyl of

estrogens, and an electron acceptor at C-2 to give a donor-acceptor fluorophore. Addnl. substituents at C-5 and C-11 provide addnl. bulk that improves receptor binding affinity without distorting the planar conjugated system. The tetrahydrochrysene core was prepd. by an acyloin condensation of .alpha.-alkyl m-methoxyhydrocinnamate esters, followed by a double dehydrative cyclization. The cis and trans isomers of the alkyl substituted systems could be sepd. and their stereochem. confirmed by x-ray crystallog. anal.; the trans isomer has the higher receptor binding affinity, and the deriv. with Et substituents at C-5 and C-11 has the best affinity. The donor-acceptor systems were prepd. by functional group manipulations on one of the arom. methoxy groups: conversion to the trifluoromethanesulfonate was followed by a palladium-mediated Me carbonylation to give the acetyl deriv. and methoxycarbonylation to give the ester. The ester was further converted to the amide and nitrile. The nitro compd. was prepd. by nitration of a protio system, itself prepd. by hydrogenolysis of the trifluoromethanesulfonate. These tetrahydrochrysenes provide a favorable combination of estrogen receptor binding affinity and long wavelength, high quantum yield fluorescence which makes them useful as fluorescent ligands for the estrogen receptor.

ST tetrahydrochrysene fluorescent ligand estrogen receptor; stilbene chromophore tetrahydrochrysene; conformation tetrahydrochrysene estrogen receptor

IT Fluorescence
(of tetrahydrochrysene ligands for the estrogen receptor)

IT Chromophores and Chromophoric systems
(stilbene, in tetrahydrochrysene ligands for the estrogen receptor)

IT Condensation reaction
(acyloin, in prepn. of fluorescent tetrahydrochrysene ligands for the estrogen receptor)

IT Receptors
RL: RCT (Reactant)
(estrogen, fluorescent tetrahydrochrysene ligands)

IT Estrogens
RL: RCT (Reactant)
(receptors, fluorescent tetrahydrochrysene ligands)

IT 133-13-1, Diethyl ethylmalonate 2163-48-6, Diethyl propylmalonate
RL: RCT (Reactant)
(condensation of, with (chloromethyl)anisole)

IT 824-98-6, m-(Chloromethyl)anisole
RL: RCT (Reactant)
(condensation of, with di-Et ethyl- and propylmalonates)

IT 138090-26-3
RL: RCT (Reactant)
(dimerization of)

IT 6099-04-3, m-Methoxycinnamic acid
RL: RCT (Reactant)
(hydrogenation of)

IT 138090-09-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and carbonylation of)

IT 138090-00-3P 138090-01-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization by polyphosphoric acid)

IT 71505-81-2P 138089-97-1P 138089-98-2P 138089-99-3P
138090-07-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization by toluenesulfonic acid)

IT **138089-93-7P 138089-94-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)

IT 18930-99-9P 138090-02-5P 138090-03-6P 138090-04-7P
138090-05-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and demethylation by boron tribromide)

IT 138090-12-7P 138090-15-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and demethylation of)

IT 138090-10-5P 138128-48-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and detriflation of)
IT 10516-71-9P, 3-(m-Methoxyphenyl)propionic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)
IT 138090-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and nitration of)
IT 62007-42-5P 138089-95-9P 138089-96-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and silylation of)
IT 138090-08-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and triflation of)
IT 138090-06-9P 138090-11-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 138090-17-2P 138090-18-3P 138090-19-4P 138090-20-7P
138090-21-8P 138090-22-9P 138090-23-0P 138090-24-1P
138090-25-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as fluorescent ligand for the estrogen receptor)
IT 138090-13-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., demethylation, and amidation of)
IT 138090-14-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., demethylation, and dehydration of)
IT 50704-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., silylation, and methylation of)

=> d 19 37 all

L9 ANSWER 37 OF 106 CA COPYRIGHT 1998 ACS
AN 115:114819 CA
TI Synthesis of racemic (S)-(+)- or (R)-(-)-[methyl-11C]amphetamine
AU Gee, Antony; Laangstroem, Bengt
CS Inst. Chem., Univ. Uppsala, Uppsala, 751 21, Swed.
SO Acta Chem. Scand. (1991), 45(4), 431-5
CODEN: ACHSE7; ISSN: 0904-213X
DT Journal
LA English
CC 31-2 (Alkaloids)
AB (.+-.)-[methyl-11C]amphetamine (I) was prepd. by alkylation of PhCH2CH(CO2Me)2 with 11CH3I to give di-Me 2-benzyl-2-([11C]methyl)malonate which was hydrolyzed with NaOH and decarboxylated to produce 2-benzyl-[3-11C]propionic acid (II). Conversion of II into I was achieved via the Schmidt reaction. Enantiomerically pure I were obtained by the preparative LC sepn. of the (+)- or (-)-10-camphorsulfonamide derivs. of (.+-.)-I with a total decay-cor. radiochem. yield of 7%. The position of labeling was confirmed by a 13C synthesis using the same reaction pathway, and anal. by 13C NMR spectroscopy.
ST amphetamine carbon labeled
IT 135154-83-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and Schmidt reaction of)
IT 135154-84-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and resoln. of)
IT 135154-85-7P 135268-27-8P 135268-28-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **132629-17-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., hydrolysis, and decarboxylation of)
IT 4227-95-6, Methyl-13C iodide 54245-42-0, Methyl-11C iodide

RL: RCT (Reactant)
(reaction of, with benzylmalonate)
IT 49769-78-0, Dimethyl 2-benzylmalonate
RL: RCT (Reactant)
(reaction of, with labeled Me iodide)

=> d 19 51 all

L9 ANSWER 51 OF 106 CA COPYRIGHT 1998 ACS
AN 110:153913 CA
TI Process for the production of (.mu.)-2-(3-aminobenzyl)butyric acid, an intermediate for the contrast agent iopanoic acid
IN Palecek, Jaroslav; Pis, Jaroslav; Londyn, Miroslav; Borovicka, Milos; Lukac, Juraj; Dedek, Vaclav; Mostecky, Jiri
PA Czech.
SO Czech., 5 pp.
CODEN: CZXXA9
PI CS 246794 B1 871215
AI CS 85-2883 850419
DT Patent
LA Czech
IC ICM C07C101-447
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 8
AB (.+-.)-3-H2NC6H4CH2CHEtCO2H (I), a key intermediate for the radiog. contrast medium iopanoic acid, is prepd. from 3-O2NC6H4CHO or 3-O2NC6H4CO2R (II; R = Me, Et) in 5 steps. Redn. of II (R = Me) by NaAlH2(OCH2CH2OMe)2 in PhMe at 5-10.degree. gave 87.4% 3-O2NC6H4CH2OH, which (33.5 g) was refluxed with azeotropic-concn. HBr for 3 h to give 32 g 3-O2NC6H4CH2Br (III). EtCH(CO2Et)2 (43.7 g) was refluxed with 5.34 g powd. Na in PhMe, and the resultant Na salt was treated with 50 g III and the mixt. refluxed for 5 h to give 57.2 g 3-O2NC6H4CH2CEt(CO2Et)2. This (15 g) was hydrogenated over PtO2 in EtOH to give 12.6 g corresponding amino diester, which (9.6 g) was sapond. by KOH in refluxing aq. EtOH and decarboxylated by HCl in the same soln. to give 3.92 g I after recrystn. from C6H6-heptane.
ST aminobenzylbutyrate prepn intermediate iopanoic acid; radiog contrast medium intermediate prepn
IT 133-13-1, Diethyl ethylmalonate 18995-13-6, Diethyl ethylmalonate sodium salt 112303-24-9, Dimethyl ethylmalonate sodium salt
RL: RCT (Reactant)
(condensation of, with nitrobenzyl halides)
IT 99-61-6, 3-Nitrobenzaldehyde 618-95-1, Methyl 3-nitrobenzoate 618-98-4, Ethyl 3-nitrobenzoate
RL: RCT (Reactant)
(hydride redn. of)
IT 96-83-3, Iopanoic acid
RL: RCT (Reactant)
(intermediate for, prepn. of (aminobenzyl)butyryic acid as)
IT 619-23-8P, 3-Nitrobenzyl chloride 3958-56-3P, 3-Nitrobenzyl iodide 3958-57-4P, 3-Nitrobenzyl bromide
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with dialkyl ethylmalonate)
IT 619-25-0P, 3-Nitrobenzyl alcohol
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to halides)
IT **118688-44-1P 118688-45-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenation of)
IT **118688-46-3P 118688-47-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon.-decarboxylation of)
IT 118688-42-9P, (.+-.)-2(3-Aminobenzyl)butyric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, from nitrobenzaldehyde or nitrobenzoate, as iopanoic acid intermediate)

=> d 19 52 all

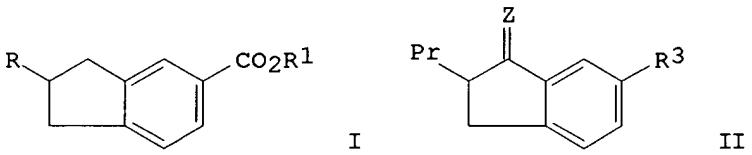
L9 ANSWER 52 OF 106 CA COPYRIGHT 1998 ACS
AN 110:82286 CA
TI Preparation of methylphenylalkanal and -alkanol derivatives as perfume constituents
IN Hafner, Walter; Gebauer, Helmut; Regiert, Marlies; Friedrich, Wilhelm; Markl, Erich
PA Consortium fuer Elektrochemische Industrie G.m.b.H., Fed. Rep. Ger.
SO Ger. Offen., 6 pp.
CODEN: GWXXBX
PI DE 3703584 A1 880818
AI DE 87-3703584 870206
DT Patent
LA German
IC ICM C07C033-20
ICS C07C047-228; A61K007-46; C11D003-50
ICA A61K007-50; C08K005-05; C08K005-07
CC 62-5 (Essential Oils and Cosmetics)
Section cross-reference(s): 25
AB 2-Methyl-3-(3-methylphenyl)propanal (I), 2-methyl-3-(3,5-dimethylphenyl)propanal, 2-methyl-3-(3-methylphenyl)-1-propanol (II), 2-methyl-3-(3,5-dimethylphenyl)-1-propanol, 1-(3-methylphenyl)-2-methyl-3-butanol, and 1-(3,5-dimethylphenyl)-2-methyl-3-butanol are prepd. as perfume constituents. 3-Methylbenzaldehyde (123 g) was condensed with 62 g EtCHO in 7.5 g KOH-contg. 240 mL EtOH to give 2-(3-methylbenzylidene)propionaldehyde, which was hydrogenated over Pd/activated charcoal in cyclohexane to give I and II.
ST alkanal methylphenyl prepn perfume constituent; perfume methylphenylalkanal methylphenylalkanol prepn; alkanol methylphenyl prepn perfume constituent
IT Perfumes and Essences
(phenylalkanal and phenylalkanol for, prepn. of)
IT 620-19-9, 3-Methylbenzyl chloride 2745-54-2, 3,5-Dimethylbenzyl chloride
RL: RCT (Reactant)
(Grignard reaction of, with chloroacetone)
IT 78-95-5
RL: RCT (Reactant)
(Grignard reaction of, with dimethylbenzyl chloride)
IT 5779-95-3, 3,5-Dimethylbenzaldehyde
RL: RCT (Reactant)
(Reformatskii reaction of, with Me bromopropionate)
IT 5445-17-0, Methyl 2-bromopropionate
RL: RCT (Reactant)
(Reformatskii reaction of, with benzaldehyde derivs.)
IT 123-38-6, Propionaldehyde, reactions
RL: RCT (Reactant)
(condensation of, with methylbenzaldehyde)
IT 620-23-5, 3-Methylbenzaldehyde
RL: BIOL (Biological study)
(condensation of, with propionaldehyde)
IT 119052-85-6
RL: RCT (Reactant)
(cyclization of, epoxide from)
IT **94430-87-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)
IT 119052-89-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydride redn. of)
IT 119052-82-3P 119052-86-7P 119052-91-4P
RL: PREP (Preparation); RCT (Reactant)
(prepn. and redn. of)
IT 119052-83-4P 119052-84-5P 119052-87-8P 119052-88-9P
119052-90-3P 119052-92-5P
RL: PREP (Preparation)
(prepn. of, as perfume constituent)
IT 620-19-9, 3-Methylbenzyl chloride

RL: RCT (Reactant)
(reaction of, with di-Et methylmalonate)

IT 78-93-3, Methyl ethyl ketone, reactions 609-08-5, Diethyl methylmalonate
RL: RCT (Reactant)
(reaction of, with methylbenzyl chloride)

=> d 19 63 all

L9 ANSWER 63 OF 106 CA COPYRIGHT 1998 ACS
AN 103:123192 CA
TI 2-Alkylindan-5-carboxylic acid derivatives as liquid crystals
PA Kanto Chemical Co., Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
PI JP 60069055 A2 850419 Showa
AI JP 83-176986 830927
DT Patent
LA Japanese
IC ICM C07C063-49
ICS C07C069-773; C07C121-52; C09K019-32
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75
GI



I II

AB Title derivs. I (R = C1-10 alkyl; R1 = H, C6H4R2; R2 = cyano, C1-10 alkyl, alkoxy), useful in nematic liq. crystal display devices, are prepd. Thus, PhCH2CHPrCO2H (prepd. from di-Et malonate, PrBr, and PhCH2Cl) was heated in the presence of polyphosphoric acid to give 94.3% II (Z = O; R3 = H) (III). Clemmensen redn. of III gave 82.5% II (R3 = H, Z = H2) which was acetylated with AcCl to give 93.6% II (R3 = COMe; Z = H2) and oxidized by NaOCl to g give 70.3% I (R = Pr, R1 = H). The latter compd. was chlorinated and treated with 2.8 g 4-EtOC6H4OH to give 2.3 g I (R = Pr; R1 = C6H4OEt-4).

ST nematic liq crystal indancarboxylate prepn; phenylpropionic acid cyclization

IT Liquid crystals
(alkyl indancarboxylates)

IT 106-94-5
RL: RCT (Reactant)
(alkylation by, malonate)

IT 109-65-9 110-53-2 111-25-1 629-04-9
RL: RCT (Reactant)
(alkylation by, of malonate)

IT 105-53-3
RL: RCT (Reactant)
(alkylation of)

IT 622-62-8 645-56-7 767-00-0
RL: RCT (Reactant)
(esterification by, of indancarbonyl chloride)

IT 64624-93-7P 66324-75-2P 66325-07-3P 66325-36-8P 66359-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)

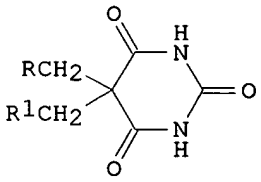
IT 133-08-4P 607-83-0P 2163-48-6P 5398-10-7P 6065-59-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzylation of)

IT 5668-19-9P 6008-22-6P 15327-02-3P 15327-07-8P 98191-23-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)

IT 15326-95-1P 15326-96-2P 15374-23-9P 42361-33-1P
98190-97-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)
IT 98191-01-6P 98191-02-7P 98191-03-8P 98191-04-9P 98191-24-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn. of)
IT 76937-26-3P 92013-10-0P 98190-98-8P 98190-99-9P 98191-00-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)
IT 98191-09-4P 98191-10-7P 98191-11-8P 98191-12-9P 98191-13-0P
98191-14-1P 98191-15-2P 98191-16-3P 98191-17-4P 98191-18-5P
98191-19-6P 98191-20-9P 98191-21-0P 98191-22-1P 98191-26-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 98191-05-0P 98191-06-1P 98191-07-2P 98191-08-3P 98191-25-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., chlorination, and esterification of)
IT 100-44-7, reactions
RL: RCT (Reactant)
(reaction of, with malonate)

=> d l9 76 all

L9 ANSWER 76 OF 106 CA COPYRIGHT 1998 ACS
AN 93:95235 CA
TI Flexible and rigid molecules - an anticonvulsant without sedative properties
AU Qazi, T. U.; Askam, V.; Sewell, R. D.
CS Fac. Pharm., Univ. Al-Faateh, Tripoli, Libya
SO Libyan J. Sci. (1979), 9B, 79-84
CODEN: LBJSAP; ISSN: 0368-7481
DT Journal
LA English
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
GI



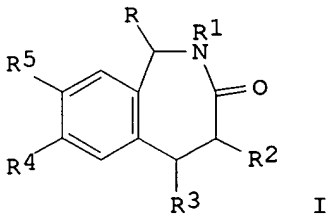
I

AB The barbiturates I (RR1 = o-C6H4; R = Ph, R1 = H) were prepd. from RCH2(R1CH2)C(CO2Et)2 and urea. 2-Indanylcarbonylurea (II) was also prepd. I and II were less active than phenobarbitone in the antileptozol test. I (RR1 = o-C6H4) was less active than I (R = Ph, R1 = H). The activity of I (RR1 = o-C6H4) was more persistent than that of the others. I (RR1 = o-C6H4) and II had similar levels of activity. I (R = Ph, R1 = H) was devoid of sedative activity at anticonvulsant levels.
ST indanespirobarbituric acid prepn pharmacol; barbiturate benzylmethyl prepn pharmacol; anticonvulsant benzylmethylbarbbiturate; structure activity anticonvulsant barbiturate
IT Anticonvulsants and Antiepileptics
(benzylmethylbarbiturate)
IT Molecular structure-biological activity relationship
(anticonvulsant, of barbiturate derivs.)
IT 609-08-5
RL: RCT (Reactant)
(benzylation of)
IT 50-01-1
RL: RCT (Reactant)

(cyclocondensation of, with indanedicarboxylate)
IT 57-13-6, reactions
RL: RCT (Reactant)
(cyclocondensation of, with malonate derivs.)
IT 74547-23-2P 74547-24-3P 74547-25-4P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anticonvulsant activity of)
IT **55114-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation of, with urea)
IT 66014-45-7
RL: RCT (Reactant)
(reaction of, with urea)

=> d 19 80 all

L9 ANSWER 80 OF 106 CA COPYRIGHT 1998 ACS
AN 88:152456 CA
TI Pharmaceutical 1,2,4,5-tetrahydro-3H-2-benzazepin-3-ones
IN Croisier, Paul; Rodriguez, Ludovic
PA UCB S. A., Belg.
SO Ger. Offen., 51 pp.
CODEN: GWXXBX
PI DE 2733868 780202
PRAI GB 76-31846 760730
DT Patent
LA German
IC C07D223-16
CC 27-22 (Heterocyclic Compounds (One Hetero Atom))
GI



I

AB The title compds. I [R = H, Ph; R1 = H, alkyl (optionally, substituted by OH, CN, alkoxy, H2NCO, NH2, tetrahydropyranyloxy, etc.) alkenyl, acyl; R2 = H, C1-4 alkyl; R3 = H, C1-4 alkyl, Ph; R4 = H, halogen, C1-4 alkoxy; R5 = H, halogen, C1-4 alkyl) were prepd. by several methods. Thus, 2,4-(NC)ClC6H3CH2CH2CHMeCO2Me was hydrogenated over Raney Ni in MeOH soln. to give 26% I (R = R1 = R3 = R4 = H, R2 = Me, R5 = Cl). I are useful for treatment of mental disorders and hypoxia; animal test results were tabulated.
ST psychotropic benzazepinone prepn; hypoxia benzazepinone
IT Psychotropics
(tetrahydrobenzazepinone)
IT 506-96-7 14077-58-8
RL: RCT (Reactant)
(acetylation by, of benzazepinone deriv.)
IT 74-88-4, reactions 75-03-6 78-77-3 106-95-6, reactions 107-14-2 107-30-2 109-54-6 110-53-2 627-42-9
RL: RCT (Reactant)
(alkylation by, of benzazepinone deriv.)
IT 57854-49-6
RL: RCT (Reactant)
(cyclocondensation of, with benzaldehyde)
IT 100-52-7, reactions
RL: RCT (Reactant)
(cyclocondensation of, with phenylpropionamide)
IT 7782-44-7, biological studies

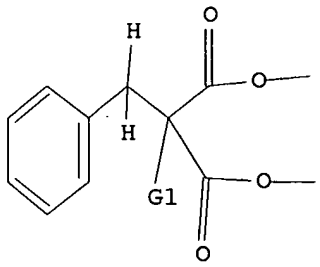
RL: BIOL (Biological study)
(defficiency of, tetrahydrobenzazepinones in treatment of)
IT 5411-56-3
RL: RCT (Reactant)
(halogenation of)
IT 30525-89-4
RL: RCT (Reactant)
(hydroxymethylation by, of propionamide deriv.)
IT 7474-19-3
RL: RCT (Reactant)
(hydroxymethylation of)
IT 39220-74-1P 66191-74-0P 66191-75-1P 66191-76-2P 66191-77-3P
66191-78-4P 66191-79-5P 66191-80-8P 66191-81-9P 66191-82-0P
66191-83-1P 66191-84-2P 66192-26-5P 66192-30-1P 66219-16-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)
IT **66192-10-7P** 66192-11-8P **66192-12-9P**
66192-13-0P 66192-14-1P 66192-15-2P **66192-16-3P**
66192-17-4P 66192-18-5P **66192-19-6P** **66192-20-9P**
66192-21-0P 66192-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)
IT 15115-58-9P 66191-98-8P 66191-99-9P 66192-00-5P 66192-01-6P
66192-02-7P 66192-03-8P 66192-04-9P 66192-05-0P 66192-06-1P
66192-07-2P 66192-08-3P 66192-09-4P 66192-29-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)
IT 17724-38-8P 66191-62-6P 66191-63-7P 66191-64-8P 66191-65-9P
66191-66-0P 66191-67-1P 66191-68-2P 66191-69-3P 66191-70-6P
66191-71-7P 66191-72-8P 66191-73-9P 66192-27-6P 66192-31-2P
66192-32-3P 66192-33-4P 66192-34-5P 66192-35-6P 66192-36-7P
66192-37-8P 66192-38-9P 66192-39-0P 66192-40-3P 66192-41-4P
66192-42-5P 66192-43-6P 66192-44-7P 66192-45-8P 66192-46-9P
66192-47-0P 66192-48-1P 66192-49-2P 66192-50-5P 66192-51-6P
66192-52-7P 66192-53-8P 66192-54-9P 66192-55-0P 66192-56-1P
66192-57-2P 66192-58-3P 66192-59-4P 66192-60-7P 66192-61-8P
66192-62-9P 66192-63-0P 66192-64-1P 66192-65-2P 66192-66-3P
66192-67-4P 66192-68-5P 66192-69-6P 66192-70-9P 66192-71-0P
66192-72-1P 66192-73-2P 66192-74-3P 66192-75-4P 66192-76-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 66191-85-3P 66191-86-4P 66191-87-5P 66191-88-6P 66191-89-7P
66191-90-0P 66191-91-1P 66191-92-2P 66191-93-3P 66191-94-4P
66191-95-5P 66191-96-6P 66191-97-7P 66192-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, and reaction with copper cyanide)
IT 3433-80-5P 62384-31-0P 66192-23-2P 66192-24-3P 66192-25-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, and reaction with malonate esters)
IT 96-34-4 107-13-1, reactions 17739-45-6
RL: RCT (Reactant)
(reaction of, with benzazepinone deriv.)
IT 544-92-3
RL: RCT (Reactant)
(reaction of, with bromophenylpropionate derivs.)
IT 609-08-5
RL: RCT (Reactant)
(reaction of, with halobenzyl halides)

=> d 9 91 all

L11 HAS NO ANSWERS
'ALL ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
data. (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
data.

SDA ----- All Structure DAta (image, attributes, connection table and map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:.

L2 STR



G1 Me,Et,n-Pr

Structure attributes must be viewed using STN Express query preparation.
L5 SCR 1839
L8 128 SEA FILE=REGISTRY SSS FUL L2 NOT L5
L9 106 SEA FILE=CA L8
L10 1713 SEA FILE=CA ARYLPROPANOL? OR BENZENEPROPANOL? OR PHENYLPROPANOL?
L11 0 SEA FILE=CA L9 AND L10

=> d 19 91 all

L9 ANSWER 91 OF 106 CA COPYRIGHT 1998 ACS
AN 81:152082 CA
TI Synthesis of biologically active compounds on the basis of substituted malonates
AU Adzhibekyan, A. S.; Ter-Zakharyan, Z.; Paronikyan, G. M.; Markaryan, E. A.
CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Erevan, USSR
SO Arm. Khim. Zh. (1974), 27(5), 434-40
CODEN: AYKZAN
DT Journal
LA Russian
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
GI For diagram(s), see printed CA Issue.
AB PhNHCONH2 condensed with 4,3-R(MeO)C6H3CH2CR1(CO2Et)2 (R = MeO, EtO; R1 = H, Me, Et, Pr, Bu, allyl) in EtOH contg. NaOEt to give the corresponding barbiturates I. 3,4-R(MeO)C6H3-CH2CR1(CO2Et)2 (R = H, MeO; R1 = Me, Et, Pr, Bu, allyl) underwent successive hydrolysis-decarboxylation, treatment with SOCl2, and condensation with 6-amino-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid to give the penicillins II. The mutagenic activities of I and antibiotic activities of II were detd.
ST antibiotic penicillin; mutagen barbiturate; malonate phenylurea condensation; barbiturate benzylphenyl; penicillin phenylacetyl
IT Mutagens
(benzylbarbiturates as)
IT Penicillin, hydrocinnamoyl derivs.
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(antibiotic activity of)
IT 105-53-3 133-08-4 609-08-5 2049-80-1 2163-48-6
RL: RCT (Reactant)
(condensation reaction of, with alkoxybenzyl chlorides)
IT 551-16-6
RL: RCT (Reactant)
(condensation reaction of, with hydrocinnamate derivs.)
IT 7306-46-9 53979-18-3
RL: RCT (Reactant)
(condensation reaction of, with malonate derivs.)

IT 53979-47-8P 53979-48-9P 53979-49-0P 53979-50-3P 53979-51-4P
53979-52-5P 53979-53-6P 53979-54-7P 53979-55-8P 53979-56-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antibiotic activity of)
IT 53979-19-4P **53979-20-7P 53979-21-8P**
53979-22-9P 53979-23-0P 53979-24-1P 53979-25-2P
53979-26-3P 53979-27-4P 53979-28-5P
53979-29-6P 53979-30-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis-decarboxylation of)
IT 53979-37-6P 53979-38-7P 53979-39-8P 53979-40-1P 53979-41-2P
53979-42-3P 53979-43-4P 53979-44-5P 53979-45-6P 53979-46-7P
54021-37-3P 54021-38-4P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and mutagenic activity of)
IT 18622-70-3P 52427-11-9P 53979-31-0P 53979-32-1P 53979-33-2P
53979-34-3P 53979-35-4P 53979-36-5P 54021-35-1P 54021-36-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with penicillin deriv.)

=> d 19 87 all

L9 ANSWER 87 OF 106 CA COPYRIGHT 1998 ACS
AN 83:205954 CA
TI Acyl-substituted phenyl propionic acids
IN Houlihan, William J.; Nadelson, Jeffrey
PA Sandoz-Wander, Inc., USA
SO U.S., 6 pp.
CODEN: USXXAM
PI US 3907878 750923
AI US 73-333893 730220
DT Patent
LA English
IC C07C
NCL 260515000R
CC 25-17 (Noncondensed Aromatic Compounds)
AB 4-(Me3CCO)C6H4(CH2)2CO2H (I) was prepd. by refluxing 4-(Me3CCO)C6H4CH2CH(CO2Et)2 (II) with aq. KOH and EtOH. Methylation of II with MeI followed by decarboxylation gave 4-(Me3CCO)C6H4CH2CHMeCO2H (III). II was prepd. by the reaction of the Grignard reagent from 4-MeC6H4Br with Me3CCOCl, followed by bromination, to give 4-BrCH2C6H4COCMe3, which reacted with H2C(CO2Et)2 and NaH in AcNMe2. I and III were useful as hypolipidemic agents; animal tests were described.
ST hypolipidemic pivaloylphenylpropionate; phenylpropionate pivaloyl
IT Anticholesteremics
((pivaloylphenyl)propionic acids)
IT Lipids
RL: RCT (Reactant)
(lowering of, in blood, by (pivaloylphenyl)propionic acids)
IT 3282-30-2
RL: RCT (Reactant)
(Grignard reaction of, with bromotoluene)
IT 106-38-7
RL: RCT (Reactant)
(Grignard reaction of, with pivaloyl chloride)
IT 74-88-4
RL: RCT (Reactant)
(alkylation by, of diethyl benzylmalonate)
IT 30314-44-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and bromination of)
IT 57373-96-3P **57373-97-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)
IT 57373-98-5P 57373-99-6P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
IT 52449-32-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, and reaction with diethyl malonate)
IT 105-53-3
RL: RCT (Reactant)
(reaction of, with bromopivaloyltoluene)

=> d l9 83 all

L9 ANSWER 83 OF 106 CA COPYRIGHT 1998 ACS
AN 86:16505 CA
TI Synthesis of isocoumarins via indanones
AU Carter, Rachel H.; Colyer, Roger M.; Hill, Robert A.; Staunton, James
CS Univ. Chem. Lab., Univ. Cambridge, Cambridge, Engl.
SO J. Chem. Soc., Perkin Trans. 1 (1976), (13), 1438-41
CODEN: JCPRB4
DT Journal
LA English
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 26
GI For diagram(s), see printed CA Issue.
AB Reaction of 5,3-R(MeO)C6H3CHO (R = MeO, H) with di-Et malonate gave 5,3-R(MeO)C6H3CH:C(CO2Et)2 which on sequential hydrogenation, methylation, sapon., and decarboxylation gave 5,3-R(MeO)C6H3CH2CHMeCO2H. Acid-catalyzed cyclization of the latter compd. gave the indanones I which on hydroxylation and NaIO4 oxidn. or ozonolysis of the corresponding trifluoroacetate gave the isocoumarins II.
ST indanone ring enlargement; isocoumarin
IT Ring enlargement
(of indanones to isocoumarins)
IT 61227-50-7P 61227-51-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)
IT 16123-39-0P **61227-49-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and decarboxylation of)
IT 5292-53-5P 6771-54-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenation of)
IT 61227-52-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydroxylation of)
IT 5859-68-7P 61227-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methylation of)
IT 61227-54-1P 61227-55-2P 61227-56-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ozonolysis of)
IT 61227-53-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ring enlargement of)
IT **16123-38-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
IT 830-54-6P 18110-66-2P 60848-62-6P 61227-57-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 591-31-1 7311-34-4
RL: RCT (Reactant)
(reaction with diethyl malonate)
IT 105-53-3
RL: RCT (Reactant)
(reaction with methoxybenzaldehydes)

=> log y

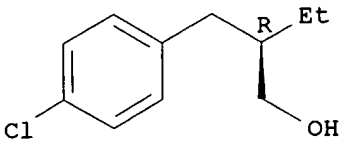
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	72.62	199.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.39	-5.39

STN INTERNATIONAL LOGOFF AT 15:59:44 ON 05 JUN 1998

L11 ANSWER 30 OF 34 REGISTRY COPYRIGHT 1998 ACS
RN 179951-12-3 REGISTRY
CN Benzenepropanol, 4-chloro-.beta.-ethyl-, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H15 Cl O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



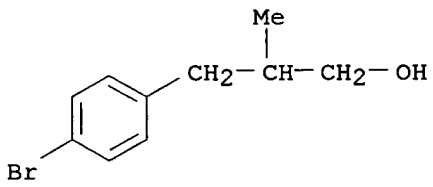
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German

=> d 25 sub bib

L11 ANSWER 25 OF 34 REGISTRY COPYRIGHT 1998 ACS
RN 186497-72-3 REGISTRY
CN Benzenepropanol, 4-bromo-.beta.-methyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Methyl-3-(4-bromophenyl)-1-propanol
CN 4-Bromo-.beta.-methylbenzenepropanol
FS 3D CONCORD
MF C10 H13 Br O
SR CA
LC STN Files: CA, CAPLUS



3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 127:50629 CA
TI Preparation of substituted biphenylsulfonamide derivatives as endothelin antagonists
IN Marugesan, Natesan; Barrish, Joel C.; Lloyd, John
PA Bristol-Myers Squibb Company, Japan
SO Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
PI JP 09124620 A2 970513 Heisei
AI JP 96-262859 961003
PRAI US 95-60007032 951011
DT Patent
LA Japanese

REFERENCE 2

AN 126:343561 CA
TI Preparation of N-isoxazolyl-biphenylsulfonamides as endothelin antagonists
IN Murugesan, Natesan; Barrish, Joel C.; Lloyd, John
PA Bristol-Myers Squibb Company, USA
SO Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
PI EP 768305 A1 970416
DS R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
AI EP 96-116095 961008
PRAI US 95-7032 951011
DT Patent
LA English

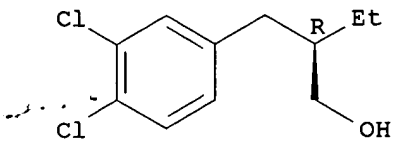
REFERENCE 3

AN 126:144291 CA
TI N-pyrazinyl-2-phenyl-3-pyridinesulfonamides and analogs endothelin receptor antagonists
IN Bradbury, Robert Hugh; Butlin, Roger John; James, Roger
PA Zeneca Limited, UK
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
PI WO 9640681 A1 961219
DS W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 96-GB1295 960603
PRAI GB 95-11507 950607
GB 95-19666 950927
DT Patent
LA English

=> d 29 sub bib

L11 ANSWER 29 OF 34 REGISTRY COPYRIGHT 1998 ACS
RN 179951-14-5 REGISTRY
CN Benzenepropanol, 3,4-dichloro-.beta.-ethyl-, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H14 Cl2 O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German

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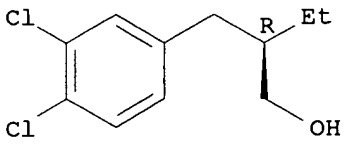
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	237.13	237.28

STN INTERNATIONAL LOGOFF AT 14:02:53 ON 05 JUN 1998

=> d ide bib abs 1-9

L11 ANSWER 1 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 179951-14-5 REGISTRY
CN Benzenepropanol, 3,4-dichloro-.beta.-ethyl-, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H14 Cl2 O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

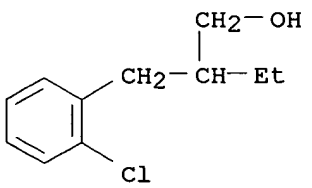


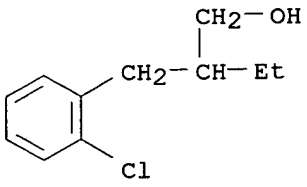
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German
AB RCH2CR1R2(CH2)nOH and RCH:CR1(CH2)nOH [R = (un)substituted Ph; R1 = H, (O- or S-interrupted) alkyl; R2 = (O- or S-interrupted) alkyl; n = 1 or 2] were prepd. Data for biol. activity of title compds. were given.

L11 ANSWER 2 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 179951-13-4 REGISTRY
CN Benzenepropanol, 2-chloro-.beta.-ethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H15 Cl O
SR CA
LC STN Files: CA, CAPLUS





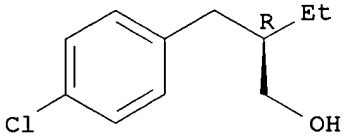
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German
AB RCH2CR1R2(CH2)nOH and RCH:CR1(CH2)nOH [R = (un)substituted Ph; R1 = H, (O- or S-interrupted) alkyl; R2 = (O- or S-interrupted) alkyl; n = 1 or 2] were prepd. Data for biol. activity of title compds. were given.

L11 ANSWER 3 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 179951-12-3 REGISTRY
CN Benzenepropanol, 4-chloro-.beta.-ethyl-, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H15 Cl O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



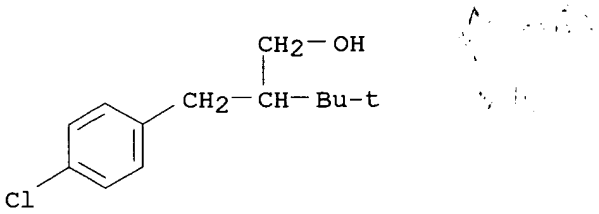
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German
AB RCH2CR1R2(CH2)nOH and RCH:CR1(CH2)nOH [R = (un)substituted Ph; R1 = H, (O- or S-interrupted) alkyl; R2 = (O- or S-interrupted) alkyl; n

= 1 or 2] were prepd. Data for biol. activity of title compds. were given.

L11 ANSWER 4 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 107021-89-6 REGISTRY
CN Benzenepropanol, 4-chloro-.beta.-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H19 Cl O
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

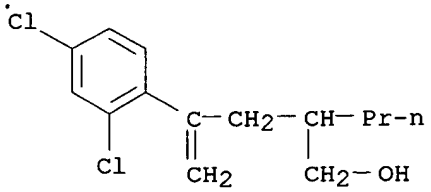


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 106:115193 CA
TI 1-Acylimidazoles with broad-spectrum fungicidal activity
AU Manabe, Akio; Kirino, Osamu; Funaki, Yuji; Hisada, Yoshio; Takano, Hirotaka; Tanaka, Shizuya
CS Takarazuka Res. Cent., Sumitomo Chem. Co., Ltd., Takarazuka, 665, Japan
SO Agric. Biol. Chem. (1986), 50(12), 3215-17
CODEN: ABCHA6; ISSN: 0002-1369
DT Journal
LA English
AB The fungicidal activity of six 1-[2-(4-chlorobenzyl)-3,3-dimethylbutanoyl]azoles and related compds. were evaluated against powdery mildew of barley and gray mold of cucumber in pot expts. 1-[2-(4-Chlorobenzyl)-3,3-dimethylbutanoyl]imidazole (I) [89371-98-2] exhibited both curative and preventive activity against Erysiphe graminis and Botrytis cinerea. Replacement of the imidazole moiety of I with 1,2,4-triazole or introduction of a Me group at the 2- or 4-position of the imidazole moiety markedly decreased activity. The steric property around the 3-N atom of the imidazole ring is important for high activity and the 1-acylimidazole skeleton appears to be important for broad spectrum fungicidal activity.

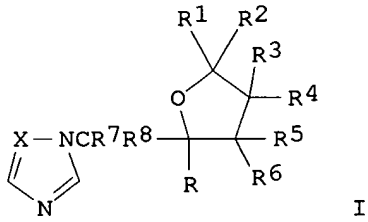
L11 ANSWER 5 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 89058-47-9 REGISTRY
CN Benzenebutanol, 2,4-dichloro-.delta.-methylene-.beta.-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H18 Cl2 O
LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

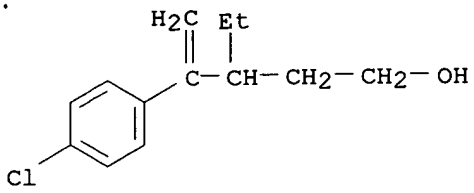
AN 100:103338 CA
TI Triazole and imidazole derivatives
IN Marchington, Anthony Frank; Lewis, Timothy; Clough, John Martin; Worthington, Paul Anthony; Griffin, David Alan; Dalziel, John
PA Imperial Chemical Industries PLC, UK
SO Brit. UK Pat. Appl., 57 pp.
CODEN: BAXXDU
PI GB 2115408 A1 830907
AI GB 83-95 830105
PRAI GB 82-3707 820209
GB 82-11290 820419
GB 82-13652 820511
GB 82-31263 821102
DT Patent
LA English
GI



I

AB The plant growth regulation and fungicidal title compds. I [R = (un)substituted aryl, aralkyl, alkyl; R1-R6 = H, (un)substituted alkyl, cycloalkyl, aralkyl, or Ph; R7, R8 = H, alkyl, (un)substituted Ph, X = CH, N] and their acid addn. salts and metal complexes were prepd. Thus, p-ClC6H4C(:CH2)CH2CH2CH(OH)CH2CH2Me prepd. in 5 steps from 4-ClC6H4CHO and H2C:CHCO2Me, was brominated with Br to give 2-(4-chlorophenyl)-3-(bromethyl)-5-propyltetrahydrofuran, which was treated with 1,2,4-triazole sodium salt to give I (R = 4-ClC6H4, R1 = Pr, R2-R8 = H, X = N) (II). At 0.05% II completely controlled Butrytis cinereo on apples. At 4.0 kg/ha I (R = 2-FC6H4, R1 = Me, R2-R8 = H, X = N) reduced the height of barley to 77% that of control.

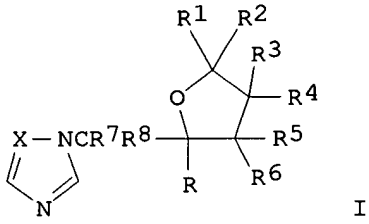
L11 ANSWER 6 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 89058-41-3 REGISTRY
CN Benzenebutanol, 4-chloro-.gamma.-ethyl-.delta.-methylene- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H17 Cl O
LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

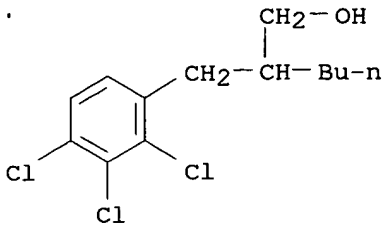
AN 100:103338 CA
TI Triazole and imidazole derivatives
IN Marchington, Anthony Frank; Lewis, Timothy; Clough, John Martin; Worthington, Paul Anthony; Griffin, David Alan; Dalziel, John
PA Imperial Chemical Industries PLC, UK
SO Brit. UK Pat. Appl., 57 pp.
CODEN: BAXXDU
PI GB 2115408 A1 830907
AI GB 83-95 830105
PRAI GB 82-3707 820209
GB 82-11290 820419
GB 82-13652 820511
GB 82-31263 821102
DT Patent
LA English
GI



I

AB The plant growth regulation and fungicidal title compds. I [R = (un)substituted aryl, aralkyl, alkyl; R1-R6 = H, (un)substituted alkyl, cycloalkyl, aralkyl, or Ph; R7, R8 = H, alkyl, (un)substituted Ph, X = CH, N] and their acid addn. salts and metal complexes were prepd. Thus, p-ClC6H4C(:CH2)CH2CH2CH(OH)CH2CH2Me prepd. in 5 steps from 4-ClC6H4CHO and H2C:CHCO2Me, was brominated with Br to give 2-(4-chlorophenyl)-3-(bromethyl)-5-propyltetrahydrofuran, which was treated with 1,2,4-triazole sodium salt to give I (R = 4-ClC6H4, R1 = Pr, R2-R8 = H, X = N) (II). At 0.05% II completely controlled Butrytis cinereo on apples. At 4.0 kg/ha I (R = 2-FC6H4, R1 = Me, R2-R8 = H, X = N) reduced the height of barley to 77% that of control.

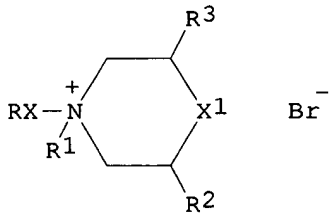
L11 ANSWER 7 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 85705-73-3 REGISTRY
CN Benzenepropanol, .beta.-butyl-2,3,4-trichloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H17 Cl3 O
LC STN Files: CA, CAPLUS, USPATFULL



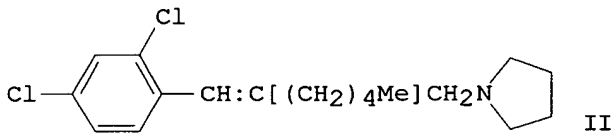
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 99:122286 CA
TI Fungicides containing phenylpropylammonium salt and methods for control of fungi
IN Buschmann, Ernst; Zeeh, Bernd; Pommer, Ernst Heinrich; Ammermann, Eberhard
PA BASF A.-G. , Fed. Rep. Ger.
SO Ger. Offen., 36 pp.
CODEN: GWXXBX
PI DE 3135592 A1 830317
AI DE 81-3135592 810909
DT Patent
LA German
GI



I



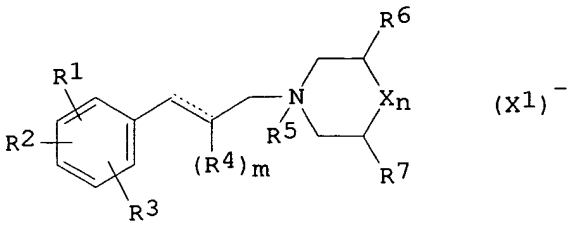
II

AB Title compds. I [R = (un)substituted Ph; R1 = alkyl, alkenyl, alkynyl, aralkyl; R2, R3 = H, alkyl, CH2OH, OH; X = alkylene, alkenylene; X1 = bond, alkylene, CO, O, S] were prepd. as fungicides. Thus, 2,4-Cl2C6H3CHO was condensed with heptanal to give 2,4-Cl2C6H3CH:C(CHO)(CH2)4Me, which was reduced to the alc., which was brominated and then condensed with pyrrolidine to give II. II was treated with CH2:CHCH2Br to give I [R = 2,4-Cl2C6H3, R1 = allyl, R3 = R4 = H, X = CH:C[(CH2)4Me]CH2, X1 = bond]. At 0.025%, I are more effective than captan against Phytophthora infestans on tomato seedlings.

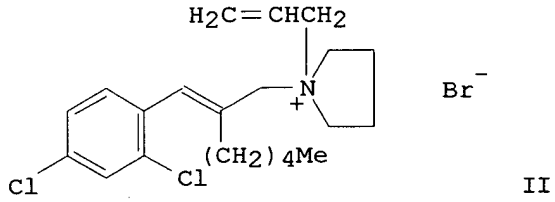
REFERENCE 2

AN 99:22341 CA
TI Fungicides containing phenylpropylammonium salts and control of fungi
IN Buschmann, Ernst; Zeeh, Bernd; Pommer, Ernst Heinrich; Ammermann, Eberhard

PA BASF A.-G. , Fed. Rep. Ger.
SO Ger. Offen., 38 pp.
CODEN: GWXXBX
PI DE 3134220 A1 830310
AI DE 81-3134220 810829
DT Patent
LA German
GI



I

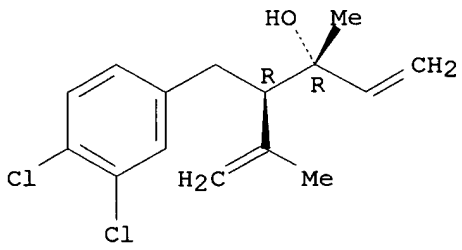


II

AB Quaternary ammonium salts I [R1, R2, R3 independently = H, (halo)alkyl, (un)substituted aryl or aralkyl, cycloalkyl, alkoxy, acyl, halo; R4 = alkyl, alkenyl, alkoxy, R5 = aliph. group, (un)substituted aralkyl; R6, R7 = H, alkyl, CH2OH, OH; X = CH2, O, S, CO, (CH2)2, CH2CHR8 (R8 = alkyl); m = 0-2; n = 0, 1; (X1) = anion non-phytotoxic acid], useful as agricultural fungicides (no data), were prepd. Pyrrolidinium salt II was prepd. in 5 steps from 2,4-Cl2C6H3CHO and Me(CH2)5CHO. Some of the I prepd. had a better fungicide activity at 0.05 than N-trichloromethylthiotetrahydrophali mide (no further information).

L11 ANSWER 8 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 67935-88-0 REGISTRY
CN Benzenepropanol, 3,4-dichloro-.alpha.-ethenyl-.alpha.-methyl-.beta.-(1-methylethenyl)-, (R*,R*)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H18 Cl2 O
LC STN Files: CA, CAPLUS

Relative stereochemistry.

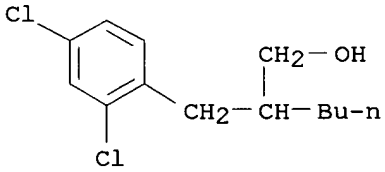


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 89:163214 CA
TI A novel method for introduction of the isoprene skeleton into chloromethylarenes and -heteroarenes via a three-step sequence involving a solvent-assisted Claisen-Cope rearrangement
AU Fujita, Yoshiji; Onishi, Takashi; Nishida, Takashi
CS Cent. Res. Lab., Kuraray Co., Ltd., Kurashiki, Japan
SO Synthesis (1978), (8), 612-14
CODEN: SYNTBF; ISSN: 0039-7881
DT Journal
LA English
AB Treatment of RCH2Cl (I, R = Ph, substituted Ph, 2-furyl, 2-thienyl) with Me2C:CHCOMe (II) and NaNH2 in liq. NH3-Et2O (1:1) gave .apprx.65-70% product, predominantly MeCOCH(CH2R)CMe:CH2 (III), whereas reaction of I with II in 55% aq. NaOH using a phase-transfer catalyst gave .apprx.80% of a mixt. of III and MeCOC(CH2R):CMe2. The Grignard reaction of III with CH2:CHBr in THF gave .apprx.80% CH2:CHCMe(OH)CH(CH2R)CMe:CH2 (IV), thermal rearrangement of which, neat, at 170-90.degree., gave 55-9% RCH2CH:CMe(CH2)3COMe (V), contg. 60-5% of E isomer; however, in the presence of 2 vols. of 1-methyl-2-pyrrolidinone at 190.degree., the rearrangement gave 78-83% V contg. 70-5% E isomer. The improved yield and selectivity is attributed to solvent assistance in the Claisen-Cope rearrangement.

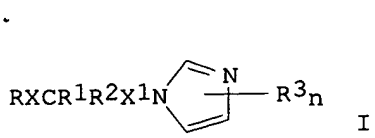
L11 ANSWER 9 OF 9 REGISTRY COPYRIGHT 1997 ACS
RN 61023-57-2 REGISTRY
CN Benzenepropanol, .beta.-butyl-2,4-dichloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H18 Cl2 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



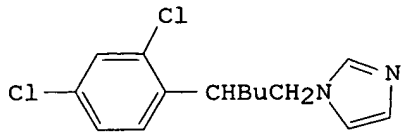
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 90:87455 CA
TI 1-Substituted aralkyl imidazoles
IN Miller, George A.; Chan, Hak-Foon
PA Rohm and Haas Co., USA
SO U.S., 23 pp.
CODEN: USXXAM
PI US 4118461 781003
AI US 75-547291 750205
DT Patent
LA English
GI



I

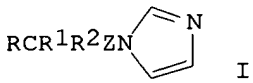


II

AB Imidazoles I (R = aryl, furyl, thienyl; CR1R2 = C3-8 cycloalkanediyl; R3 = C1-4 alkyl, halogen, NO2; X, X1 = bond, C1-5 alkylene; n = 0-3) (104 compds.) were prepd. Thus treating 2,4-Cl2C6H3CH2CO2Et with IBu gave 2,4-Cl2C6H3CHBuCO2Et, which was reduced to the alc., mesylated, and treated with imidazole to give II. At 300 ppm II gave .gtoreq.97% control of Erysiphe polygoni on beans.

REFERENCE 2

AN 90:87450 CA
TI 1-Substituted aralkyl imidazoles
IN Miller, George A.; Owen, Ronald P.
PA Rohm and Haas Co., USA
SO U.S., 22 pp.
CODEN: USXXAM
PI US 4115578 780919
AI US 75-547291 750205
DT Patent
LA English
GI

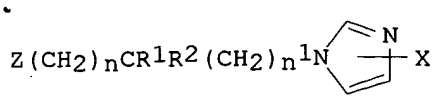


I

AB 1-(.omega.-Phenylalkyl)imidazoles [R or R2 = H, Ph, halophenyl, alkylphenyl, alkoxyphenyl, nitrophenyl, aminophenyl, (methylthio)phenyl, (trihalomethyl)phenyl; R1 = H, alkyl, alkenyl, aralkyl; Z = C1-5 alkylene] (104 compds.) were prepd. and showed fungicidal activity. Thus, alkylating 2,4-Cl2C6H3CH2CO2Et with BuI and then redn. gave 2,4-Cl2C6H3CHBuCH2OH, which was O-mesylated; treating imidazole with the mesylate gave I (R = 2,4-Cl2C6H3, R1 = Bu, R2 = H, Z = CH2), which at 300 ppm. gave 90-100% control of various test fungi on beans.

REFERENCE 3

AN 86:1093 CA
TI Imidazole fungicides
IN Miller, George Allen; Carley, Harold E.; Chan, Hak-Foon
PA Rohm and Haas Co., USA
SO Ger. Offen., 145 pp.
CODEN: GWXXBX
PI DE 2604047 760916
PRAI US 75-547291 750205
DT Patent
LA German
GI



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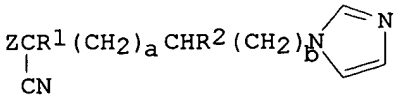
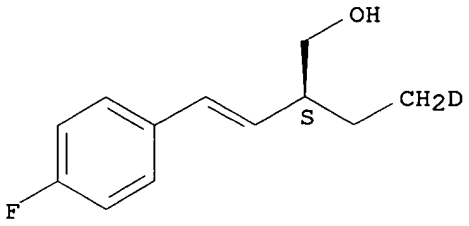


II

AB The imidazole derivs. I (Z = halophenyl, heterocylic radical, etc; n and n2 = 0, 1, or 2; R1 = lower alkyl, R2 = H or Me; X = H, 2-Me, 4-NO2, etc) and II (Z = Ph, alkylphenyl, halophenyl etc; R1 = H, alkyl, etc; R2 = H, Pr, or Ph; a and b = 0, 1, 2, 3, or 4) and I and II salts and adducts are fungicides. Thus, 300 ppm 1-[.beta.-(2,4-dichlorophenyl)heryl]imidazole [58831-30-4] completely controlled Helminthosporium teres on barley, Grysiphe polygoni on bean, and Puccinia recondita on wheat, in pot expts. The synthesis of I and II is given.

L11 ANSWER 1 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 190185-59-2 REGISTRY
CN 3-Buten-1-ol, 2-(ethyl-2-d)-4-(4-fluorophenyl)-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H14 D F O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



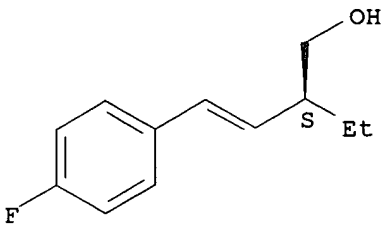
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 127:4876 CA
TI Zirconium-catalyzed enantioselective 2-aluminoethylalumination of alkenes
AU Dawson, Graham; Durrant, Charles A.; Kirk, George G.; Whitby, Richard J.
CS Dep. Chem., Univ. Southampton, Southampton, SO17 1BJ, UK
SO Tetrahedron Lett. (1997), 38(13), 2335-2338
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB Asym. 2-aluminoethylalumination of mono-substituted alkenes and 2,5-dihydrofurans catalyzed by (R,R)-ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-indenyl)zirconium (R)-1,1'-binaphth-2,2'-diolate and .eta.5-cyclopentadienyl-.eta.5-(1-neomenthyl-4,5,6,7-tetrahydroindenyl)zirconium dichloride. gave 30-99% enantiomeric excesses. The so formed organoaluminum has potential for further elaboration leading to enantiomerically enriched products.

L11 ANSWER 2 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 184047-37-8 REGISTRY
CN 3-Buten-1-ol, 2-ethyl-4-(4-fluorophenyl)-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H15 F O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

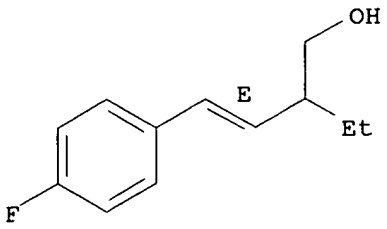
AN 127:4876 CA
TI Zirconium-catalyzed enantioselective 2-aluminoethylalumination of alkenes
AU Dawson, Graham; Durrant, Charles A.; Kirk, George G.; Whitby, Richard J.
CS Dep. Chem., Univ. Southampton, Southampton, SO17 1BJ, UK
SO Tetrahedron Lett. (1997), 38(13), 2335-2338
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB Asym. 2-aluminoethylalumination of mono-substituted alkenes and 2,5-dihydrofurans catalyzed by (R,R)-ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-indenyl)zirconium (R)-1,1'-binaphth-2,2'-diolate and .eta.5-cyclopentadienyl-.eta.5-(1-neomenthyl-4,5,6,7-tetrahydroindenyl)zirconium dichloride. gave 30-99% enantiomeric excesses. The so formed organoaluminum has potential for further elaboration leading to enantiomerically enriched products.

REFERENCE 2

AN 126:7439 CA
TI Catalytic asymmetric carbomagnesiation of unactivated alkenes. A new, effective, active, cheap and recoverable chiral zirconocene
AU Bell, Louise; Whitby, Richard J.; Jones, Raymond V. H.; Standen, Michael C. H.
CS Dep. Chem., The University, Southampton, SO17 1BJ, UK
SO Tetrahedron Lett. (1996), 37(39), 7139-7142
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB The ethylmagnesiation of terminal alkenes, e.g., PhNHCH2CH:CH2, catalyzed by (R,R)-ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-indenyl)zirconium (R)-1,1'-binaphth-2,2'-diolate gave low turnovers and enantioexcesses. A novel Ci sym. zirconocene dichloride CpCp'ZrCl2 (Cp = C5H5, Cp' = 1-neomenthyl-4,5,6,7-tetrahydroindenyl) was prepd. which gave better enantioselectivity, is cheaper to make, catalytically more active, and recoverable.

L11 ANSWER 3 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 182073-38-7 REGISTRY
CN 3-Buten-1-ol, 2-ethyl-4-(4-fluorophenyl)-, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H15 F O
SR CA
LC STN Files: CA, CAPLUS

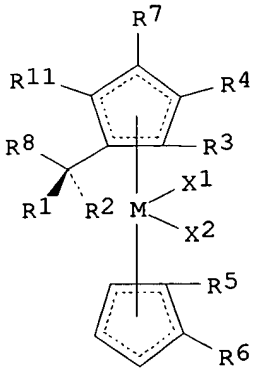
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:248112 CA
TI Chiral organometallic compounds
IN Jones, Raymond Vincent Heavon; Standen, Michael Charles Henry; Whitby, Richard John; Bell, Jane Louise
PA Zeneca Limited, UK
SO PCT Int. Appl., 45 pp.
CODEN: PIXXD2
PI WO 9625420 A1 960822
DS W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE
AI WO 96-GB264 960206
PRAI GB 95-2870 950214
DT Patent
LA English
GI



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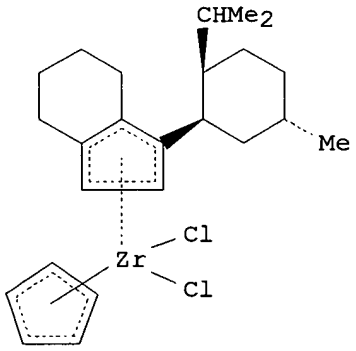


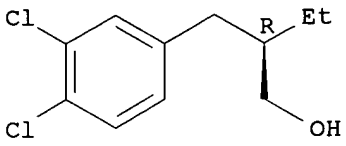
II

AB Chiral, organometallic compds. which, at a mol. level, have no C2 symmetry and comprise C to C bonds joining chiral C atoms to C atoms of cyclopentadiene rings that are nonsym. substituted are disclosed. Examples of such compds. include compds. I wherein X1 and X2 are independently groups which are removable during a chem. reaction and M is Ti, Zr or Hf. An example of a prepd. compd. is I.

L11 ANSWER 4 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 179951-14-5 REGISTRY
CN Benzenepropanol, 3,4-dichloro-.beta.-ethyl-, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H14 Cl2 O

SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

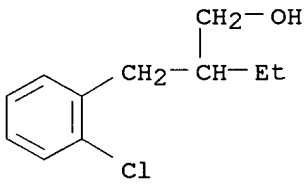


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German
AB RCH2CR1R2(CH2)nOH and RCH:CR1(CH2)nOH [R = (un)substituted Ph; R1 = H, (O- or S-interrupted) alkyl; R2 = (O- or S-interrupted) alkyl; n = 1 or 2] were prepd. Data for biol. activity of title compds. were given.

L11 ANSWER 5 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 179951-13-4 REGISTRY
CN Benzenepropanol, 2-chloro-.beta.-ethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H15 Cl O
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

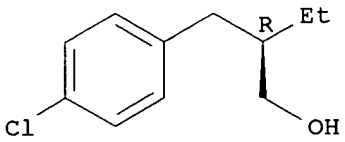
REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221

DT Patent
LA German
AB RCH2CR1R2(CH2)nOH and RCH:CR1(CH2)nOH [R = (un)substituted Ph; R1 = H, (O- or S-interrupted) alkyl; R2 = (O- or S-interrupted) alkyl; n = 1 or 2] were prepd. Data for biol. activity of title compds. were given.

L11 ANSWER 6 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 179951-12-3 REGISTRY
CN Benzenepropanol, 4-chloro-.beta.-ethyl-, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H15 Cl O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

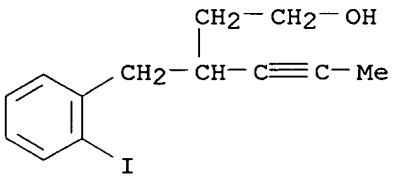


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 125:142252 CA
TI Preparation of phenylalkanols and -alk(en)ols as biocides
IN Berscheid, Ralf; Eggensperger, Heinz; Beilfus, Wolfgang; Behrends, Sabine; Puchstein, Burghard
PA Schuelke und Mayr Gmbh, Germany
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
PI DE 4447361 A1 960627
AI DE 94-4447361 941221
DT Patent
LA German
AB RCH2CR1R2(CH2)nOH and RCH:CR1(CH2)nOH [R = (un)substituted Ph; R1 = H, (O- or S-interrupted) alkyl; R2 = (O- or S-interrupted) alkyl; n = 1 or 2] were prepd. Data for biol. activity of title compds. were given.

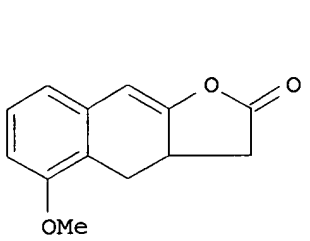
L11 ANSWER 7 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 175235-58-2 REGISTRY
CN Benzenebutanol, 2-iodo-.gamma.-1-propynyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H15 I O
SR CA
LC STN Files: CA, CAPLUS, CASREACT



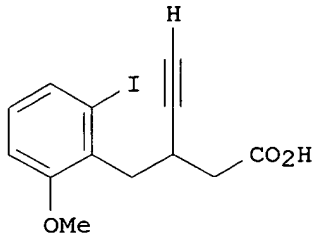
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

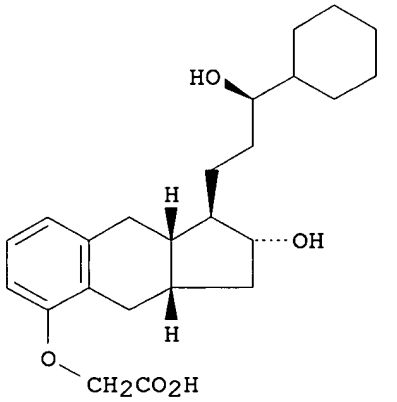
AN 125:248135 CA
TI A new route to .gamma.-arylidenebutyrolactones via a tandem carbopalladation-heterocyclization sequence: a formal synthesis of U-68,215
AU Cavicchioli, Marcello; Decortiat, Sylvie; Bouyssi, Didier; Gore, Jacques; Balme, Genevieve
CS Lab. Chim, Org. I, Univ. Claude Bernard, Villeurbanne, 69622, Fr.
SO Tetrahedron (1996), 52(35), 11463-11478
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



I



II

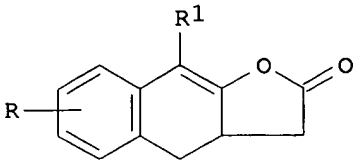


III

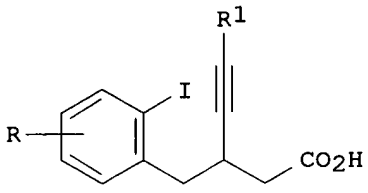
AB Benzo-annulated enol lactones, e.g. I, are obtained in good yields from pentynoic acids 3- or 5-substituted with an iodo-aryl moiety, e.g. II, by palladium-catalyzed cyclization of their potassium carboxylates. Using this approach, an efficient new route to U-68,215 (III) is described.

REFERENCE 2

AN 124:260694 CA
TI Palladium-mediated intramolecular cyclization of substituted pentynoic acids. A new route to .gamma.-arylidenebutyrolactones
AU Cavicchioli, M.; Bouyssi, D.; Gore, J.; Balme, G.
CS Laboratoire Chimie Organique I, Univ. Claude Bernard, Villeurbanne, 69622, Fr.
SO Tetrahedron Lett. (1996), 37(9), 1429-32
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
GI



I

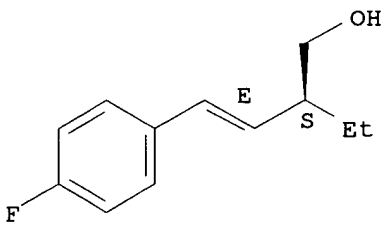


II

AB Benzo-annulated enol lactones, e.g. I (R = H, R1 = H, Me), are obtained in good yields from pentynoic acids 3- or 5-substituted, e.g. II, with an iodoaryl moiety by palladium-catalyzed cyclization of their potassium carboxylates.

L11 ANSWER 8 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 166767-92-6 REGISTRY
CN 3-Buten-1-ol, 2-ethyl-4-(4-fluorophenyl)-, [S-(E)]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H15 F O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



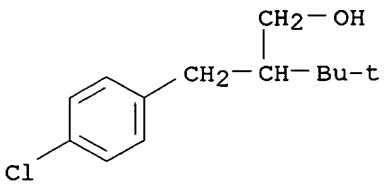
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 123:143560 CA
TI Zirconocene-catalyzed kinetic resolution of dihydrofurans
AU Visser, Michael S.; Hoveyda, Amin H.
CS Dep. Chem., Boston Coll., Chestnut Hill, MA, 02167, USA
SO Tetrahedron (1995), 51(15), 4383-94
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
AB Zirconocene-catalyzed kinetic resoln. of dihydrofurans may be affected in the presence of 10 mol% non-racemic (EBTHI)ZrCl2 [ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-indenyl)zirconium dichloride]. Transformations reported herein proceed efficiently to afford two constitutionally distinct and readily separable products with excellent levels of diastereo- and enantioselectivity. Prepn. and resoln. of the substrate furans may be carried out in a single pot.

L11 ANSWER 9 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 107021-89-6 REGISTRY
CN Benzenepropanol, 4-chloro-.beta.-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H19 Cl O

SR CA
LC STN Files: CA, CAPLUS, TOXLIT

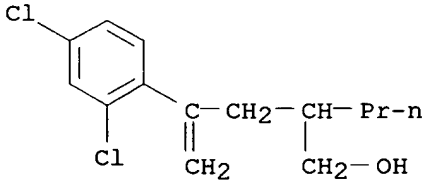


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 106:115193 CA
TI 1-Acylimidazoles with broad-spectrum fungicidal activity
AU Manabe, Akio; Kirino, Osamu; Funaki, Yuji; Hisada, Yoshio; Takano, Hirotaka; Tanaka, Shizuya
CS Takarazuka Res. Cent., Sumitomo Chem. Co., Ltd., Takarazuka, 665, Japan
SO Agric. Biol. Chem. (1986), 50(12), 3215-17
CODEN: ABCHA6; ISSN: 0002-1369
DT Journal
LA English
AB The fungicidal activity of six 1-[2-(4-chlorobenzyl)-3,3-dimethylbutanoyl]azoles and related compds. were evaluated against powdery mildew of barley and gray mold of cucumber in pot expts. 1-[2-(4-Chlorobenzyl)-3,3-dimethylbutanoyl]imidazole (I) [89371-98-2] exhibited both curative and preventive activity against Erysiphe graminis and Botrytis cinerea. Replacement of the imidazole moiety of I with 1,2,4-triazole or introduction of a Me group at the 2- or 4-position of the imidazole moiety markedly decreased activity. The steric property around the 3-N atom of the imidazole ring is important for high activity and the 1-acylimidazole skeleton appears to be important for broad spectrum fungicidal activity.

L11 ANSWER 10 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 89058-47-9 REGISTRY
CN Benzenebutanol, 2,4-dichloro-.delta.-methylene-.beta.-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H18 Cl2 O
LC STN Files: CA, CAPLUS, USPATFULL

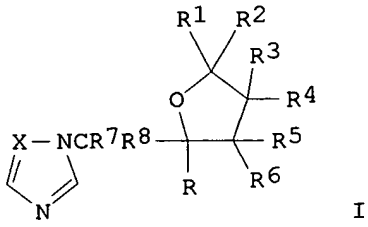


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 100:103338 CA

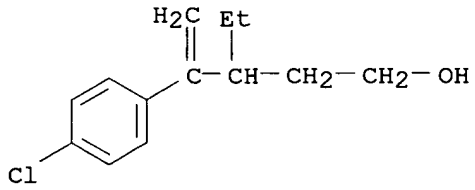
TI Triazole and imidazole derivatives
IN Marchington, Anthony Frank; Lewis, Timothy; Clough, John Martin; Worthington, Paul Anthony; Griffin, David Alan; Dalziel, John
PA Imperial Chemical Industries PLC, UK
SO Brit. UK Pat. Appl., 57 pp.
CODEN: BAXXDU
PI GB 2115408 A1 830907
AI GB 83-95 830105
PRAI GB 82-3707 820209
GB 82-11290 820419
GB 82-13652 820511
GB 82-31263 821102
DT Patent
LA English
GI



I

AB The plant growth regulation and fungicidal title compds. I [R = (un)substituted aryl, aralkyl, alkyl; R1-R6 = H, (un)substituted alkyl, cycloalkyl, aralkyl, or Ph; R7, R8 = H, alkyl, (un)substituted Ph, X = CH, N] and their acid addn. salts and metal complexes were prepd. Thus, p-ClC6H4C(:CH2)CH2CH2CH(OH)CH2CH2Me prepd. in 5 steps from 4-ClC6H4CHO and H2C:CHCO2Me, was brominated with Br to give 2-(4-chlorophenyl)-3-(bromethyl)-5-propyltetrahydrofuran, which was treated with 1,2,4-triazole sodium salt to give I (R = 4-ClC6H4, R1 = Pr, R2-R8 = H, X = N) (II). At 0.05% II completely controlled Butrytis cinereo on apples. At 4.0 kg/ha I (R = 2-FC6H4, R1 = Me, R2-R8 = H, X = N) reduced the height of barley to 77% that of control.

L11 ANSWER 11 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 89058-41-3 REGISTRY
CN Benzenebutanol, 4-chloro-.gamma.-ethyl-.delta.-methylene- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H17 Cl O
LC STN Files: CA, CAPLUS, USPATFULL

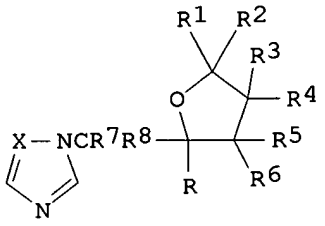


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 100:103338 CA

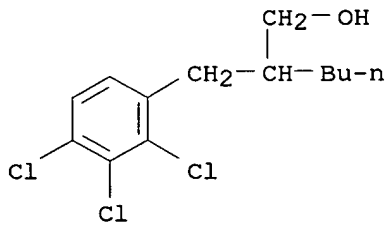
TI Triazole and imidazole derivatives
IN Marchington, Anthony Frank; Lewis, Timothy; Clough, John Martin; Worthington, Paul Anthony; Griffin, David Alan; Dalziel, John
PA Imperial Chemical Industries PLC, UK
SO Brit. UK Pat. Appl., 57 pp.
CODEN: BAXXDU
PI GB 2115408 A1 830907
AI GB 83-95 830105
PRAI GB 82-3707 820209
GB 82-11290 820419
GB 82-13652 820511
GB 82-31263 821102
DT Patent
LA English
GI



I

AB The plant growth regulation and fungicidal title compds. I [R = (un)substituted aryl, aralkyl, alkyl; R1-R6 = H, (un)substituted alkyl, cycloalkyl, aralkyl, or Ph; R7, R8 = H, alkyl, (un)substituted Ph, X = CH, N] and their acid addn. salts and metal complexes were prepd. Thus, p-ClC6H4C(:CH2)CH2CH2CH(OH)CH2CH2Me prepd. in 5 steps from 4-ClC6H4CHO and H2C:CHCO2Me, was brominated with Br to give 2-(4-chlorophenyl)-3-(bromethyl)-5-propyltetrahydrofuran, which was treated with 1,2,4-triazole sodium salt to give I (R = 4-ClC6H4, R1 = Pr, R2-R8 = H, X = N) (II). At 0.05% II completely controlled Butrytis cinereo on apples. At 4.0 kg/ha I (R = 2-FC6H4, R1 = Me, R2-R8 = H, X = N) reduced the height of barley to 77% that of control.

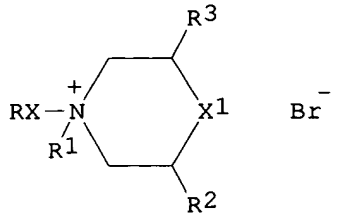
L11 ANSWER 12 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 85705-73-3 REGISTRY
CN Benzenepropanol, .beta.-butyl-2,3,4-trichloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H17 Cl3 O
LC STN Files: CA, CAPLUS, USPATFULL



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 99:122286 CA
TI Fungicides containing phenylpropylammonium salt and methods for control of fungi
IN Buschmann, Ernst; Zeeh, Bernd; Pommer, Ernst Heinrich; Ammermann, Eberhard
PA BASF A.-G. , Fed. Rep. Ger.
SO Ger. Offen., 36 pp.
CODEN: GWXXBX
PI DE 3135592 A1 830317
AI DE 81-3135592 810909
DT Patent
LA German
GI



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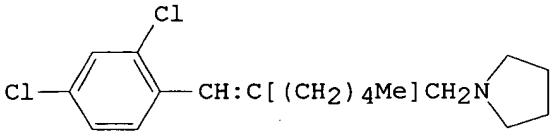
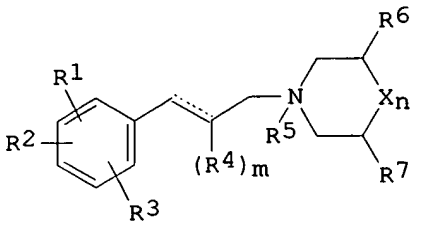


II

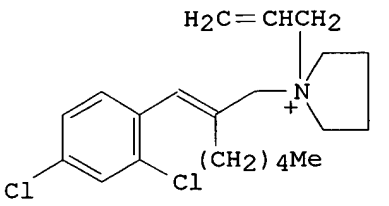
AB Title compds. I [R = (un)substituted Ph; R1 = alkyl, alkenyl, alkynyl, aralkyl; R2, R3 = H, alkyl, CH2OH, OH; X = alkylene, alkenylene; X1 = bond, alkylene, CO, O, S] were prepd. as fungicides. Thus, 2,4-Cl2C6H3CHO was condensed with heptanal to give 2,4-Cl2C6H3CH:C(CHO)(CH2)4Me, which was reduced to the alc., which was brominated and then condensed with pyrrolidine to give II. II was treated with CH2:CHCH2Br to give I [R = 2,4-Cl2C6H3, R1 = allyl, R3 = R4 = H, X = CH:C[(CH2)4Me]CH2, X1 = bond]. At 0.025%, I are more effective than captan against Phytophthora infestans on tomato seedlings.

REFERENCE 2

AN 99:22341 CA
TI Fungicides containing phenylpropylammonium salts and control of fungi
IN Buschmann, Ernst; Zeeh, Bernd; Pommer, Ernst Heinrich; Ammermann, Eberhard
PA BASF A.-G. , Fed. Rep. Ger.
SO Ger. Offen., 38 pp.
CODEN: GWXXBX
PI DE 3134220 A1 830310
AI DE 81-3134220 810829
DT Patent
LA German
GI



I

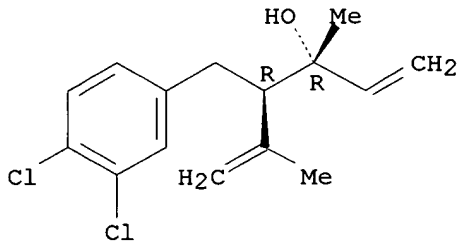


II

AB Quaternary ammonium salts I [R1, R2, R3 independently = H, (halo)alkyl, (un)substituted aryl or aralkyl, cycloalkyl, alkoxy, acyl, halo; R4 = alkyl, alkenyl, alkoxy, R5 = aliph. group, (un)substituted aralkyl; R6, R7 = H, alkyl, CH2OH, OH; X = CH2, O, S, CO, (CH2)2, CH2CHR8 (R8 = alkyl); m = 0-2; n = 0, 1; (X1) = anion non-phytotoxic acid], useful as agricultural fungicides (no data), were prepd. Pyrrolidinium salt II was prepd. in 5 steps from 2,4-Cl2C6H3CHO and Me(CH2)5CHO. Some of the I prepd. had a better fungicide activity at 0.05 than N-trichloromethylthiotetrahydrophali mide (no further information).

L11 ANSWER 13 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 67935-88-0 REGISTRY
CN Benzenepropanol, 3,4-dichloro-.alpha.-ethenyl-.alpha.-methyl-.beta.-(1-methylethenyl)-, (R*,R*)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H18 Cl2 O
LC STN Files: CA, CAPLUS

Relative stereochemistry.



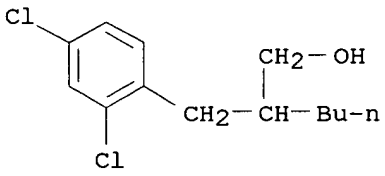
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 89:163214 CA
TI A novel method for introduction of the isoprene skeleton into chloromethylarenes and -heteroarenes via a three-step sequence involving a solvent-assisted Claisen-Cope rearrangement
AU Fujita, Yoshiji; Onishi, Takashi; Nishida, Takashi
CS Cent. Res. Lab., Kuraray Co., Ltd., Kurashiki, Japan
SO Synthesis (1978), (8), 612-14
CODEN: SYNTBF; ISSN: 0039-7881
DT Journal

LA English
AB Treatment of RCH2Cl (I, R = Ph, substituted Ph, 2-furyl, 2-thienyl) with Me2C:CHCOMe (II) and NaNH2 in liq. NH3-Et2O (1:1) gave .apprx.65-70% product, predominantly MeCOCH(CH2R)CMe:CH2 (III), whereas reaction of I with II in 55% aq. NaOH using a phase-transfer catalyst gave .apprx.80% of a mixt. of III and MeCOC(CH2R):CMe2. The Grignard reaction of III with CH2:CHBr in THF gave .apprx.80% CH2:CHCMe(OH)CH(CH2R)CMe:CH2 (IV), thermal rearrangement of which, neat, at 170-90.degree., gave 55-9% RCH2CH:CMe(CH2)3COMe (V), contg. 60-5% of E isomer; however, in the presence of 2 vols. of 1-methyl-2-pyrrolidinone at 190.degree., the rearrangement gave 78-83% V contg. 70-5% E isomer. The improved yield and selectivity is attributed to solvent assistance in the Claisen-Cope rearrangement.

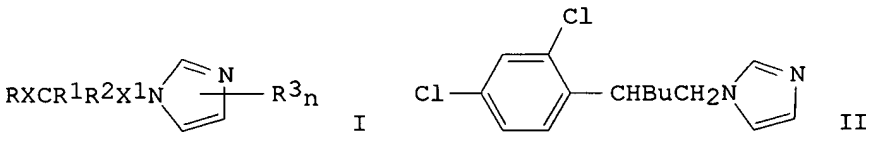
L11 ANSWER 14 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 61023-57-2 REGISTRY
CN Benzenepropanol, .beta.-butyl-2,4-dichloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H18 Cl2 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 90:87455 CA
TI 1-Substituted aralkyl imidazoles
IN Miller, George A.; Chan, Hak-Foon
PA Rohm and Haas Co., USA
SO U.S., 23 pp.
CODEN: USXXAM
PI US 4118461 781003
AI US 75-547291 750205
DT Patent
LA English
GI

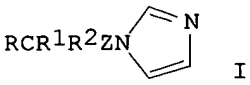


AB Imidazoles I (R = aryl, furyl, thienyl; CR1R2 = C3-8 cycloalkanediyl; R3 = C1-4 alkyl, halogen, NO2; X, X1 = bond, C1-5 alkylene; n = 0-3) (104 compds.) were prepd. Thus treating 2,4-Cl2C6H3CH2CO2Et with IBu gave 2,4-Cl2C6H3CHBuCO2Et, which was reduced to the alc., mesylated, and treated with imidazole to give II. At 300 ppm II gave .gtoreq.97% control of Erysiphe polygoni on

beans.

REFERENCE 2

AN 90:87450 CA
TI 1-Substituted aralkyl imidazoles
IN Miller, George A.; Owen, Ronald P.
PA Rohm and Haas Co., USA
SO U.S., 22 pp.
CODEN: USXXAM
PI US 4115578 780919
AI US 75-547291 750205
DT Patent
LA English
GI

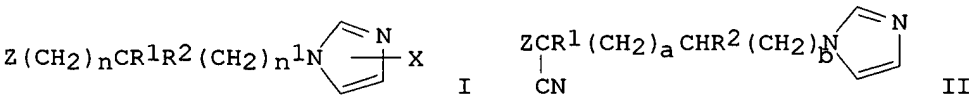


I

AB 1-(.omega.-Phenylalkyl)imidazoles [R or R2 = H, Ph, halophenyl, alkylphenyl, alkoxyphenyl, nitrophenyl, aminophenyl, (methylthio)phenyl, (trihalomethyl)phenyl; R1 = H, alkyl, alkenyl, aralkyl; Z = C1-5 alkylene] (104 compds.) were prepd. and showed fungicidal activity. Thus, alkylating 2,4-Cl2C6H3CH2CO2Et with BuI and then redn. gave 2,4-Cl2C6H3CHBuCH2OH, which was O-mesylated; treating imidazole with the mesylate gave I (R = 2,4-Cl2C6H3, R1 = Bu, R2 = H, Z = CH2), which at 300 ppm. gave 90-100% control of various test fungi on beans.

REFERENCE 3

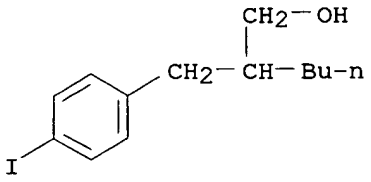
AN 86:1093 CA
TI Imidazole fungicides
IN Miller, George Allen; Carley, Harold E.; Chan, Hak-Foon
PA Rohm and Haas Co., USA
SO Ger. Offen., 145 pp.
CODEN: GWXXBX
PI DE 2604047 760916
PRAI US 75-547291 750205
DT Patent
LA German
GI



I II

AB The imidazole derivs. I (Z = halophenyl, heterocylic radical, etc; n and n2 = 0, 1, or 2; R1 = lower alkyl, R2 = H or Me; X = H, 2-Me, 4-NO2, etc) and II (Z = Ph, alkylphenyl, halophenyl etc; R1 = H, alkyl, etc; R2 = H, Pr, or Ph; a and b = 0, 1, 2, 3, or 4) and I and II salts and adducts are fungicides. Thus, 300 ppm 1-[.beta.-(2,4-dichlorophenyl)heryl]imidazole [58831-30-4] completely controlled Helminthosporium teres on barley, Grysiphe polygoni on bean, and Puccinia recondita on wheat, in pot expts. The synthesis of I and II is given.

L11 ANSWER 15 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 60075-88-9 REGISTRY
CN Benzenepropanol, .beta.-butyl-4-iodo- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-(4-Iodobenzyl)hexanol
CN 2-(p-Iodobenzyl)-1-hexanol
FS 3D CONCORD
MF C13 H19 I O
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 92:163726 CA
TI Iodoaryl carbonates for use in methods in radiography
IN Newton, Barry N.
PA Lafayette Pharmacal, Inc., USA
SO U.S., 12 pp.
CODEN: USXXAM
PI US 4175544 791127
AI US 74-501169 740828
DT Patent
LA English
AB Carbonate esters of IC6H4OH and of iodophenylalkyl alcs., useful in radiocontrast media, were prepd. Thus, iodination of PhCH2OH gave 4-IC6H4CH2OH which with COCl2 gave 4-IC6H4CH2OCOCl; this on esterification with 1-hexanol gave 4-IC6H4CH2OCO2(CH2)5Me.

REFERENCE 2

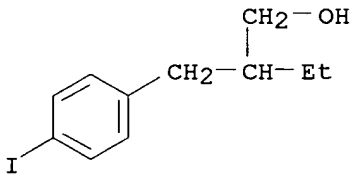
AN 87:134678 CA
TI Iodine-containing organic carbonates for use as radiographic agents
IN Newton, Barry N.
PA Lafayette Pharmacal, Inc., USA
SO U.S., 9 pp.
CODEN: USXXAM
PI US 4022814 770510
AI US 74-501169 740828
DT Patent
LA English
AB Iodoaralkyl alkyl carbonates, e.g. 4-IC6H4CHROCO2R1 (R = Me, H, etc.; R1 = Me2CH, hexyl, etc) and similar iodoaryl alkyl carbonates, useful as radiography contrast agents, were prepd. Thus, PhCH2OH was iodinated to 4-IC6H4CH2OH, which was treated with COCl2 and alcs. to give 4-IC6H4CH2OCO2R1.

REFERENCE 3

AN 85:171541 CA
TI Iodine-containing organic carbonates as investigative radiopaque compounds
AU Newton, B. N.

CS Res. Dev. Dep., Lafayette Pharmacal Inc., Lafayette, Indiana, USA
SO J. Med. Chem. (1976), 19(12), 1362-6
CODEN: JMCMAR
DT Journal
LA English
AB A series of 29 carbonate esters [ROC(:O)OR1:R = C2-C10 alkyl; R1 = p-IC6H4, m- and p-IC6H4CH2, 3,5-I2C6H3CH2, 3-NH2- and 3-AcNH-2,4,6-I3C6HCH2, p-IC6H4CH2CH2, p-IC6H4CHMe, p-IC6H4(CH2)3, p-IC6H4CHMeCH2CH2, p-IC6H4CH2CHEtCH2, p-IC6H4CH2CHBuCH2] was prepd. by reacting an alkyl chloroformate with an iodinated arom. alc. The approx. lethal dose of i.p. injections in mice was from <1 mg/kg to >15 ml/kg. As the alkyl part of the ester increased in size, toxicity increased. The m-amino and m-acetamido groups lowered toxicity of the triiodinated compds. Follow-up radiography showed complete elimination of the injected material in 1-2 weeks.

L11 ANSWER 16 OF 16 REGISTRY COPYRIGHT 1997 ACS
RN 60075-61-8 REGISTRY
CN Benzenepropanol, .beta.-ethyl-4-iodo- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-(4-Iodobenzyl)butanol
CN 2-(p-Iodobenzyl)-1-butanol
CN 2-p-Iodobenzylbutanol
FS 3D CONCORD
MF C11 H15 I O
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, RTECS*, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 92:163726 CA
TI Iodoaryl carbonates for use in methods in radiography
IN Newton, Barry N.
PA Lafayette Pharmacal, Inc., USA
SO U.S., 12 pp.
CODEN: USXXAM
PI US 4175544 791127
AI US 74-501169 740828
DT Patent
LA English
AB Carbonate esters of IC6H4OH and of iodophenylalkyl alcs., useful in radiocontrast media, were prepd. Thus, iodination of PhCH2OH gave 4-IC6H4CH2OH which with COCl2 gave 4-IC6H4CH2OCOCl; this on esterification with 1-hexanol gave 4-IC6H4CH2OCO2(CH2)5Me.

REFERENCE 2

AN 89:173397 CA
TI Structure-toxicity relationships of iodinated aromatic carbonates and related compounds
AU Newton, Barry N.
CS Res. Dev. Dep., Lafayette Pharmacal Inc., West Lafayette, Indiana,

USA
SO J. Pharm. Sci. (1978), 67(8), 1154-7
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal
LA English
AB Structure-toxicity relations of iodinated arom. carbonates, carbamates, and esters are presented. The approx. LD of i.p. injections in mice was used for toxicity detns. Increasing the alkyl portion of the mols. reduced toxicity. M-amino and m-acetamido groups also reduced toxicity. Carbonates were preferred X-ray contrast agents because of their low viscosity and more rapid elimination.

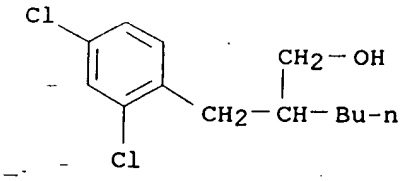
REFERENCE 3

AN 87:134678 CA
TI Iodine-containing organic carbonates for use as radiographic agents
IN Newton, Barry N.
PA Lafayette Pharmacal, Inc., USA
SO U.S., 9 pp.
CODEN: USXXAM
PI US 4022814 770510
AI US 74-501169 740828
DT Patent
LA English
AB Iodoaralkyl alkyl carbonates, e.g. 4-IC6H4CHROCO2R1 (R = Me, H, etc.; R1 = Me2CH, hexyl, etc) and similar iodoaryl alkyl carbonates, useful as radiography contrast agents, were prepd. Thus, PhCH2OH was iodinated to 4-IC6H4CH2OH, which was treated with COCl2 and alcs. to give 4-IC6H4CH2OCO2R1.

REFERENCE 4

AN 85:171541 CA
TI Iodine-containing organic carbonates as investigative radiopaque compounds
AU Newton, B. N.
CS Res. Dev. Dep., Lafayette Pharmacal Inc., Lafayette, Indiana, USA
SO J. Med. Chem. (1976), 19(12), 1362-6
CODEN: JMCMAR
DT Journal
LA English
AB A series of 29 carbonate esters [ROC(:O)OR1:R = C2-C10 alkyl; R1 = p-IC6H4, m- and p-IC6H4CH2, 3,5-I2C6H3CH2, 3-NH2- and 3-AcNH-2,4,6-I3C6HCH2, p-IC6H4CH2CH2, p-IC6H4CHMe, p-IC6H4(CH2)3, p-IC6H4CHMeCH2CH2, p-IC6H4CH2CHEtCH2, p-IC6H4CH2CHBuCH2] was prepd. by reacting an alkyl chloroformate with an iodinated arom. alc. The approx. lethal dose of i.p. injections in mice was from <1 mg/kg to >15 ml/kg. As the alkyl part of the ester increased in size, toxicity increased. The m-amino and m-acetamido groups lowered toxicity of the triiodinated compds. Follow-up radiography showed complete elimination of the injected material in 1-2 weeks.

CN Benzenepropanol, beta.-butyl-2,4-dichloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H18 Cl2 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)

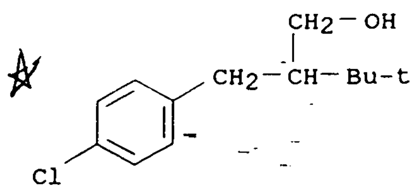


3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 90:87455 CA
TI 1-Substituted aralkyl imidazoles
IN Miller, George A.; Chan, Hak-Foon
PA Rohm and Haas Co., USA
SO U.S., 23 pp.
CODEN: USXXAM
PI US 4118461 781003
AI US 75-547291 750205
DT Patent
LA English
GI

RN 107021-89-6 REGISTRY
CN Benzenepropa[illegible] 4-chloro-.beta.-(1,1-dimethy[illegible]nyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H19 Cl O
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 106:115193 CA
TI 1-Acylimidazoles with broad-spectrum fungicidal activity
AU Manabe, Akio; Kirino, Osamu; Funaki, Yuji; Hisada, Yoshio; Takano, Hirotaka; Tanaka, Shizuya
CS Takarazuka Res. Cent., Sumitomo Chem. Co., Ltd., Takarazuka, 665, Japan
SO Agric. Biol. Chem. (1986), 50(12), 3215-17
CODEN: ABCHA6; ISSN: 0002-1369
DT Journal
LA English
AB The fungicidal activity of six 1-[2-(4-chlorobenzyl)-3,3-dimethylbutanoyl]azoles and related compds. were evaluated against powdery mildew of barley and gray mold of cucumber in pot expts. 1-[2-(4-Chlorobenzyl)-3,3-dimethylbutanoyl]imidazole (I) [89371-98-2] exhibited both curative and preventive activity against Erysiphe graminis and Botrytis cinerea. Replacement of the imidazole moiety of I with 1,2,4-triazole or introduction of a Me group at the 2- or 4-position of the imidazole moiety markedly decreased activity. The steric property around the 3-N atom of the imidazole ring is important for high activity and the 1-acylimidazole skeleton appears to be important for broad spectrum fungicidal activity.